

=> d his ful

(FILE 'HOME' ENTERED AT 09:43:24 ON 21 OCT 2005)

FILE 'HCAPLUS' ENTERED AT 09:43:52 ON 21 OCT 2005

E US20040192723/PN

L1 2 SEA ABB=ON PLU=ON US2004192723/PN
SEL RN L1

FILE 'REGISTRY' ENTERED AT 09:45:43 ON 21 OCT 2005

L2 66 SEA ABB=ON PLU=ON (100-39-0/BI OR 100-44-7/BI OR 108-68-9/BI
OR 1486-48-2/BI OR 16108-50-2/BI OR 18065-05-9/BI OR 332386-66-
0/BI OR 332386-72-8/BI OR 332386-75-1/BI OR 333796-78-4/BI OR
480-66-0/BI OR 6137-86-6/BI OR 701284-09-5/BI OR 701284-10-8/BI
OR 701284-11-9/BI OR 701284-12-0/BI OR 701284-13-1/BI OR
701284-14-2/BI OR 701284-15-3/BI OR 701284-16-4/BI OR 701284-17
-5/BI OR 701284-18-6/BI OR 701284-19-7/BI OR 701284-20-0/BI OR
701284-21-1/BI OR 701284-22-2/BI OR 701284-23-3/BI OR 701284-24
-4/BI OR 701284-26-6/BI OR 701284-27-7/BI OR 701284-28-8/BI OR
701284-29-9/BI OR 701284-30-2/BI OR 701284-31-3/BI OR 701284-32
-4/BI OR 701284-33-5/BI OR 701284-34-6/BI OR 701284-35-7/BI OR
701284-36-8/BI OR 701284-37-9/BI OR 701284-38-0/BI OR 701284-39
-1/BI OR 701284-40-4/BI OR 701284-41-5/BI OR 701284-42-6/BI OR
70424-94-1/BI OR 79831-88-2/BI OR 86-81-7/BI OR 90-24-4/BI OR
97888-80-7/BI OR 99-24-1/BI OR 120980-02-1/BI OR 219937-14-1/BI
OR 333796-77-3/BI OR 62252-08-8/BI OR 701284-25-5/BI OR
75-36-5/BI OR 765955-95-1/BI OR 765956-00-1/BI OR 765956-07-8/B
I OR 765956-13-6/BI OR 765956-20-5/BI OR 765956-21-6/BI OR
765956-22-7/BI OR 765956-23-8/BI OR 989-51-5/BI)

L3 55 SEA ABB=ON PLU=ON L2 AND NR>2

L4 55 SEA ABB=ON PLU=ON L3 AND NRS>1

L5 44 SEA ABB=ON PLU=ON L4 AND (OC5-C6 OR SC5-C6 OR NC5-C6 OR
C6-C6)/ES AND C6/ES

FILE 'HCAPLUS' ENTERED AT 09:50:52 ON 21 OCT 2005

L6 2 SEA ABB=ON PLU=ON L1 AND L5
D IALL HITSTR L6 1-2

FILE 'REGISTRY' ENTERED AT 09:54:20 ON 21 OCT 2005

L7 STR
L8 50 SEA SSS SAM L7
L9 STR L7
L10 50 SEA SSS SAM L9
L11 STR L9
L12 50 SEA SSS SAM L11
L13 STR L11
L14 50 SEA SSS SAM L13
L15 7835 SEA SSS FUL L13
SAV TEMP DAVIS690/A L15

L*** DEL STR L11

L*** DEL STR L13

D L7

L16 27633 SEA SSS FUL L7
SAV TEMP DAVIS690/A L16

L17 STR L7

L18 50 SEA SSS SAM L17

L19 STR L17

L20 144 SEA ABB=ON PLU=ON "SULFHYDRYL"

L21 9 SEA ABB=ON PLU=ON L20 NOT MAN/CI

D SCA
E MERCAPTO/CN
L22 1 SEA ABB=ON PLU=ON MERCAPTO/CN
D
L23 STR L19
L24 50 SEA SUB=L16 SSS SAM L23
L25 STR L23
L26 32 SEA SUB=L16 SSS SAM L25

FILE 'HCAPLUS' ENTERED AT 11:04:38 ON 21 OCT 2005
L27 65 SEA ABB=ON PLU=ON L26

FILE 'REGISTRY' ENTERED AT 11:04:49 ON 21 OCT 2005
L28 STR L25
L29 31 SEA SUB=L16 SSS SAM L28
L30 492 SEA SUB=L16 SSS FUL L28

FILE 'HCAPLUS' ENTERED AT 11:15:17 ON 21 OCT 2005
L31 3512 SEA ABB=ON PLU=ON L30

FILE 'REGISTRY' ENTERED AT 11:15:24 ON 21 OCT 2005
L32 303 SEA ABB=ON PLU=ON L30 AND NRS>2
L33 STR
L34 STR
L35 6 SEA SUB=L30 SSS SAM L33 AND L34
D SCA
L36 84 SEA SUB=L30 SSS FUL L33 AND L34

FILE 'HCAPLUS' ENTERED AT 11:32:28 ON 21 OCT 2005
L37 3329 SEA ABB=ON PLU=ON L36

FILE 'REGISTRY' ENTERED AT 11:32:41 ON 21 OCT 2005
L38 408 SEA ABB=ON PLU=ON L30 NOT L36

FILE 'HCAPLUS' ENTERED AT 11:33:11 ON 21 OCT 2005
L39 255 SEA ABB=ON PLU=ON L38
L40 ANALYZE PLU=ON L39 1-255 RN : 3925 TERMS
D

FILE 'REGISTRY' ENTERED AT 11:34:43 ON 21 OCT 2005
L41 1 SEA ABB=ON PLU=ON 154-23-4
D SCA

FILE 'HCAPLUS' ENTERED AT 11:35:00 ON 21 OCT 2005
L42 6352 SEA ABB=ON PLU=ON L41
S 490-46-0/REG#

FILE 'REGISTRY' ENTERED AT 11:36:21 ON 21 OCT 2005
L43 1 SEA ABB=ON PLU=ON 490-46-0/RN

FILE 'HCAPLUS' ENTERED AT 11:36:21 ON 21 OCT 2005
L44 3952 SEA ABB=ON PLU=ON L43

FILE 'REGISTRY' ENTERED AT 11:36:31 ON 21 OCT 2005
L45 1 SEA ABB=ON PLU=ON 490-46-0
D SCA
L46 1 SEA ABB=ON PLU=ON 989-51-5
D SCA
L47 0 SEA ABB=ON PLU=ON L46 AND L38

FILE 'HCAPLUS' ENTERED AT 11:40:55 ON 21 OCT 2005
L48 27 SEA ABB=ON PLU=ON L39 AND P/DT
L49 228 SEA ABB=ON PLU=ON L39 NOT L48
L50 189 SEA ABB=ON PLU=ON L49 NOT PY>2002

FILE HOME

FILE HCAPLUS

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FILE COVERS 1907 - 21 Oct 2005 VOL 143 ISS 18
FILE LAST UPDATED: 20 Oct 2005 (20051020/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 OCT 2005 HIGHEST RN 865652-03-5
DICTIONARY FILE UPDATES: 19 OCT 2005 HIGHEST RN 865652-03-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

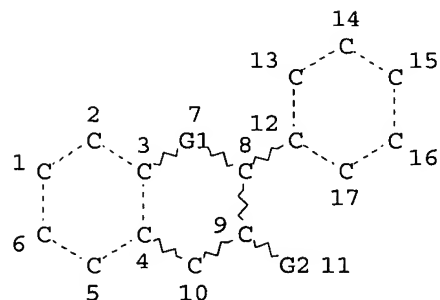
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> d que stat l48
L7 STR



NH~Ak
@18 19

Ak~N~Ak
22 @20 21

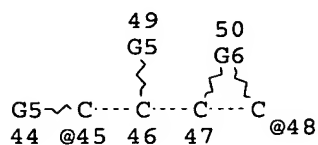
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VAR G2=O/SH/NH2/18/20
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 19
CONNECT IS E1 RC AT 21
CONNECT IS E1 RC AT 22
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

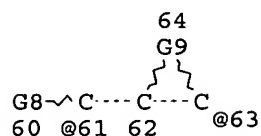
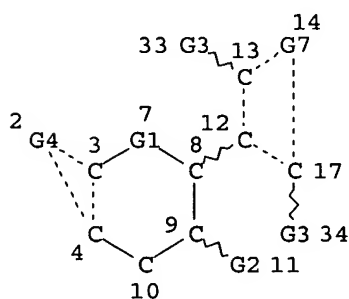
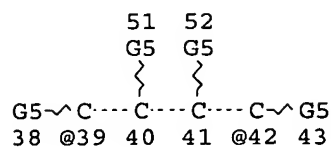
STEREO ATTRIBUTES: NONE
L16 27633 SEA FILE=REGISTRY SSS FUL L7
L28 STR

NH~Ak Ak~N~Ak O~C~O N~Ak CH~Ak Ak @
 @18 19 22 @20 21 23 24 @25 @26 27 @28 29

Ak~C~Ak O~Ak
 30 @31 32 @36 37



O~Cy
 @53 54



Page 1-A

35

Page 1-B

G8~C~C~C~G8
 55 @56 57 @58 59

Page 2-A

VAR G1=O/S/NH/CH2/26/28/31

VAR G2=SH/25/NH2/18/20

VAR G3=H/OH/35/36/X

VAR G4=39-3 42-4/45-3 48-4/48-3 45-4

VAR G5=H/OH/35/36/53

REP G6=(3-4) A

VAR G7=56-13 58-17/61-13 63-17/63-13 61-17

VAR G8=H/OH/35/X/SH/36/53

REP G9=(1-10) A

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 8

CONNECT IS E3 RC AT 9

CONNECT IS E2 RC AT 10

CONNECT IS E1 RC AT 19

CONNECT IS E1 RC AT 21

CONNECT IS E1 RC AT 22

CONNECT IS E3 RC AT 24

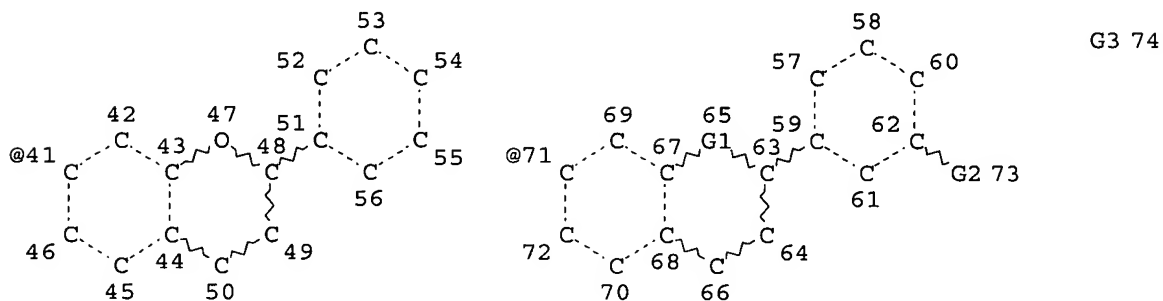
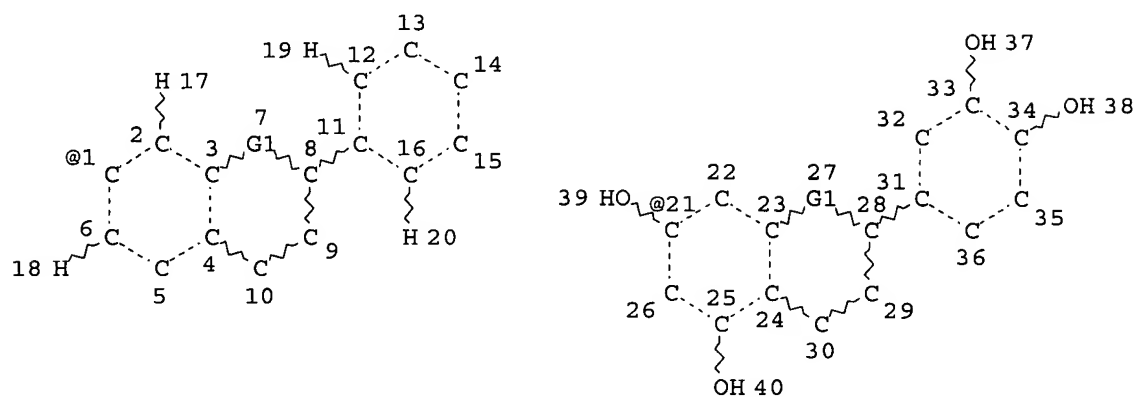
CONNECT IS E1 RC AT 27

CONNECT IS E1 RC AT 29
 CONNECT IS E1 RC AT 30
 CONNECT IS E1 RC AT 32
 CONNECT IS E1 RC AT 35
 CONNECT IS E1 RC AT 37
 CONNECT IS E1 RC AT 54
 DEFAULT MLEVEL IS ATOM
 GGCAT IS UNS AT 54
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 60

STEREO ATTRIBUTES: NONE

L30 492 SEA FILE=REGISTRY SUB=L16 SSS FUL L28
 L33 STR

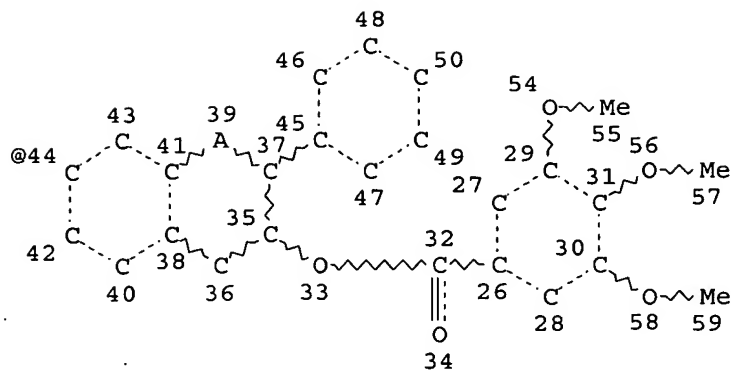


VAR G1=O/S/N/C
 VAR G2=H/OH
 VAR G3=1/21/41/71

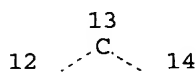
NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 74

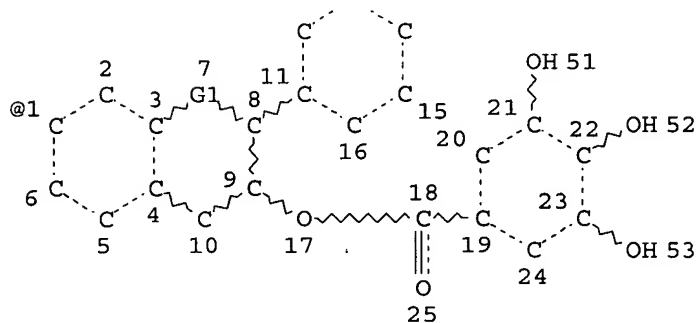
STEREO ATTRIBUTES: NONE
 L34 STR



G2 60



Page 1-A



Page 2-A

VAR G1=O/S/N/C

VAR G2=1/44

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 39

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS UNLIMITED AT 39

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 60

STEREO ATTRIBUTES: NONE

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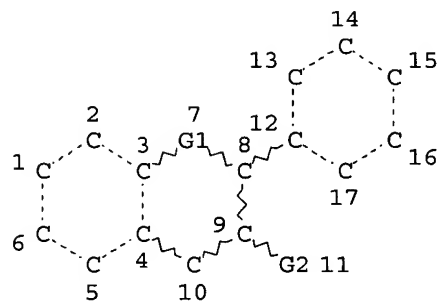
L36      84 SEA FILE=REGISTRY SUB=L30 SSS FUL L33 AND L34
L38      408 SEA FILE=REGISTRY ABB=ON  PLU=ON  L30 NOT L36
L39      255 SEA FILE=HCAPLUS ABB=ON   PLU=ON   L38
L48      27  SEA FILE=HCAPLUS ABB=ON   PLU=ON   L39 AND P/DT

```

```

=> d que stat l50
L7      STR

```



NH~Ak
@18 19

Ak~N~Ak
22 @20 21

```

VAR G1=O/S/N/C
VAR G2=O/SH/NH2/18/20
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 19
CONNECT IS E1 RC AT 21
CONNECT IS E1 RC AT 22
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

```

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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

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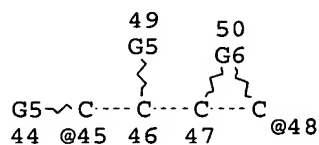
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STEREO ATTRIBUTES: NONE
L16      27633 SEA FILE=REGISTRY SSS FUL L7
L28      STR

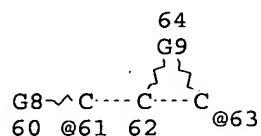
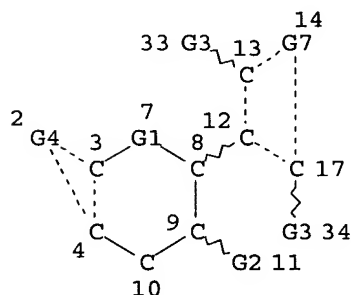
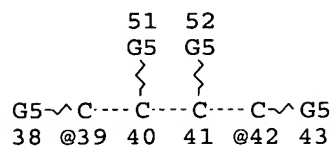
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NH~Ak Ak~N~Ak O≡C~O N~Ak CH~Ak Ak @
 @18 19 22 @20 21 23 24 @25 @26 27 @28 29

Ak~C~Ak O~Ak
 30 @31 32 @36 37



O~Cy
 @53 54



Page 1-A

35

Page 1-B

G8~C~C~C~G8
 55 @56 57 @58 59

Page 2-A

VAR G1=O/S/NH/CH2/26/28/31

VAR G2=SH/25/NH2/18/20

VAR G3=H/OH/35/36/X

VAR G4=39-3 42-4/45-3 48-4/48-3 45-4

VAR G5=H/OH/35/36/53

REP G6=(3-4) A

VAR G7=56-13 58-17/61-13 63-17/63-13 61-17

VAR G8=H/OH/35/X/SH/36/53

REP G9=(1-10) A

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 8

CONNECT IS E3 RC AT 9

CONNECT IS E2 RC AT 10

CONNECT IS E1 RC AT 19

CONNECT IS E1 RC AT 21

CONNECT IS E1 RC AT 22

CONNECT IS E3 RC AT 24

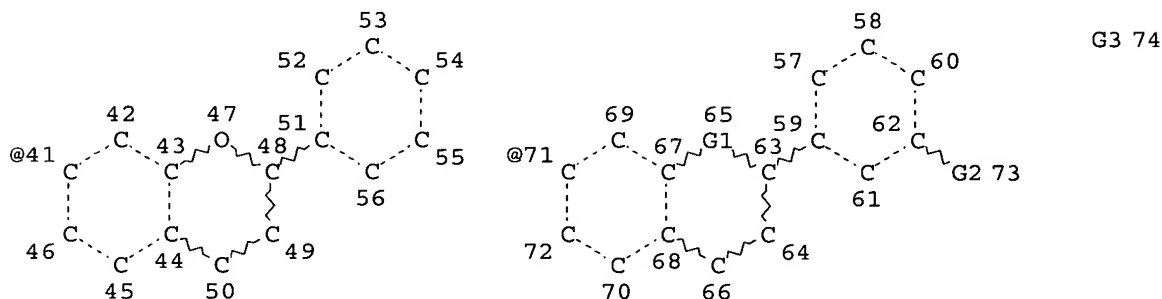
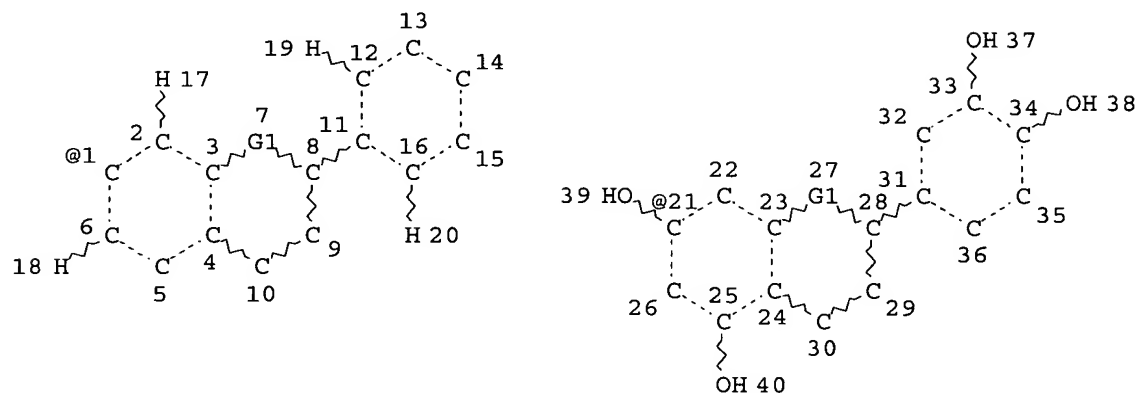
CONNECT IS E1 RC AT 27

CONNECT IS E1 RC AT 29
 CONNECT IS E1 RC AT 30
 CONNECT IS E1 RC AT 32
 CONNECT IS E1 RC AT 35
 CONNECT IS E1 RC AT 37
 CONNECT IS E1 RC AT 54
 DEFAULT MLEVEL IS ATOM
 GGCAT IS UNS AT 54
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 60

STEREO ATTRIBUTES: NONE

L30 492 SEA FILE=REGISTRY SUB=L16 SSS FUL L28
 L33 STR

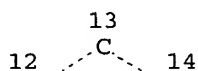
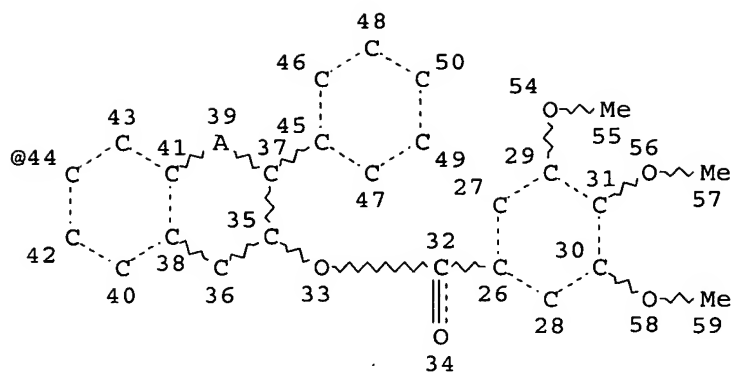


VAR G1=O/S/N/C
 VAR G2=H/OH
 VAR G3=1/21/41/71

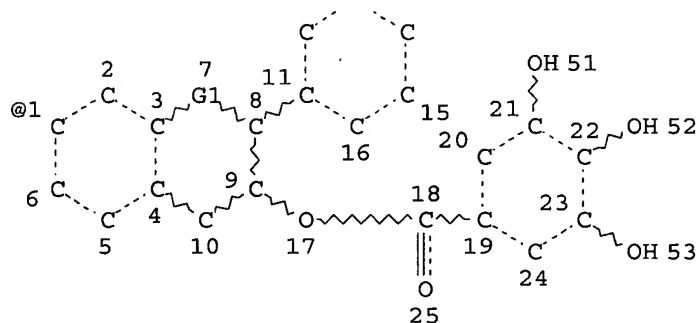
NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 74

STEREO ATTRIBUTES: NONE
 L34 STR



Page 1-A



Page 2-A

VAR G1=O/S/N/C

VAR G2=1/44

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 39

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS UNLIMITED AT 39

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 60

STEREO ATTRIBUTES: NONE

L36 84 SEA FILE=REGISTRY SUB=L30 SSS FUL L33 AND L34
 L38 408 SEA FILE=REGISTRY ABB=ON PLU=ON L30 NOT L36
 L39 255 SEA FILE=HCAPLUS ABB=ON PLU=ON L38
 L48 27 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 AND P/DT
 L49 228 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 NOT L48
 L50 189 SEA FILE=HCAPLUS ABB=ON PLU=ON L49 NOT PY>2002

=> d l48 ibib ab hitstr 1-27

L48 ANSWER 1 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2005:346877 HCAPLUS
 DOCUMENT NUMBER: 142:385968
 TITLE: Antimicrobial modified catechin compositions and
 methods of use
 INVENTOR(S): Stapleton, Paul; Uesato, Shinichi; Taylor, Peter W.
 PATENT ASSIGNEE(S): Fish, Robert, USA
 SOURCE: PCT Int. Appl., 34 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: **Patent**
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005034976	A1	20050421	WO 2003-US28750	20030912
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: WO 2003-US28750 20030912

OTHER SOURCE(S): MARPAT 142:385968

AB A catechin is modified in at least one position (most preferably in the 3-position of the C-ring) to increase its lipophilicity. Contemplated catechins are demonstrated to have significantly improved antibacterial properties, likely due to catastrophic membrane damage. 3-O-octanoyl-(-)-epicatechin exhibited significant antimicrobial effect against methicillin-resistant Staphylococcus aureus.

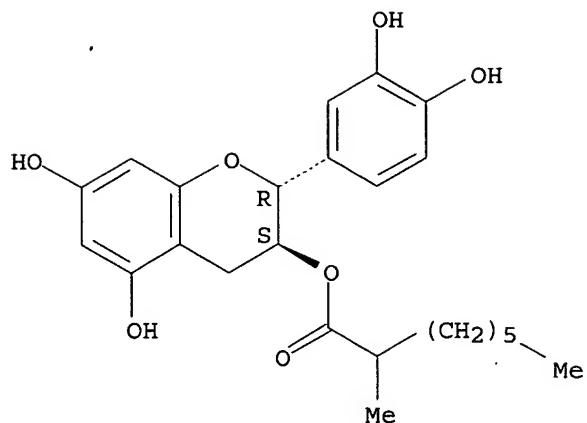
IT **662144-65-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
 (antimicrobial modified catechin compns. with increased lipophilicity)

RN 662144-65-2 HCAPLUS

CN Octanoic acid, 2-methyl-, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 71634-78-1P 71634-81-6P 71634-82-7P,
3-O-Palmitoyl-(+)-catechin 662144-60-7P 662144-61-8P
662144-62-9P 662144-63-0P 662144-64-1P

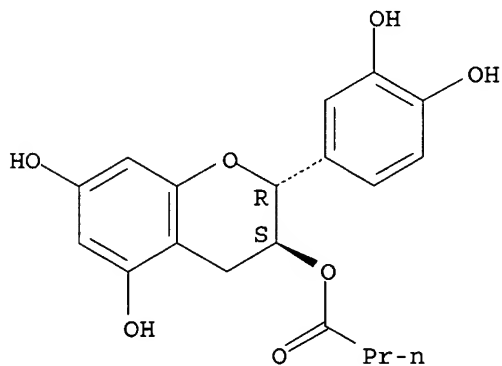
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); USES (Uses)

(bactericidal activity of; antimicrobial modified catechin compns. with
increased lipophilicity)

RN 71634-78-1 HCAPLUS

CN Butanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-
2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

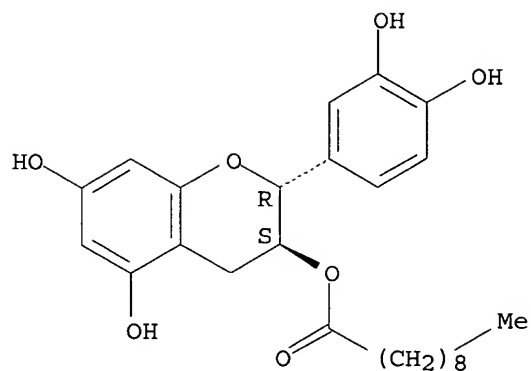
Absolute stereochemistry. Rotation (+).



RN 71634-81-6 HCAPLUS

CN Decanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-
2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

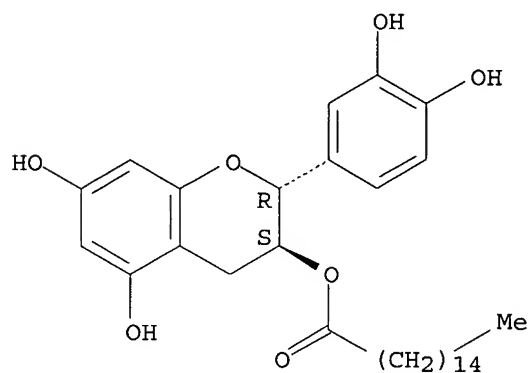
Absolute stereochemistry. Rotation (+).



RN 71634-82-7 HCAPLUS

CN Hexadecanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

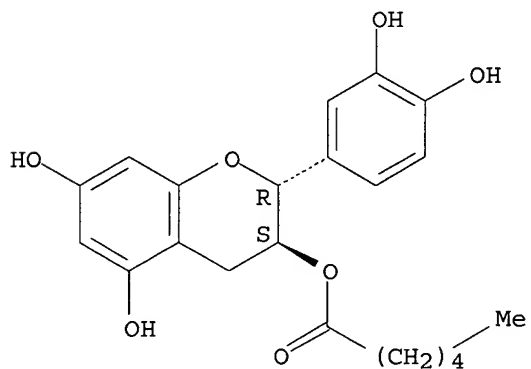
Absolute stereochemistry.



RN 662144-60-7 HCAPLUS

CN Hexanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

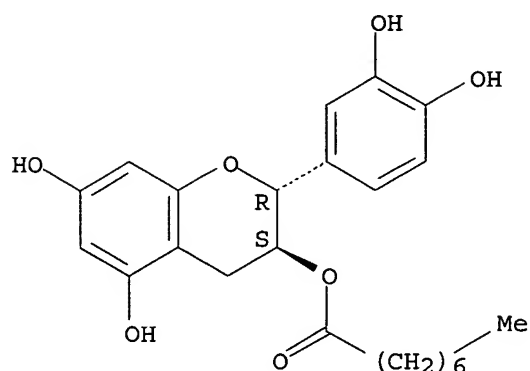


RN 662144-61-8 HCAPLUS

CN Octanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-

2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

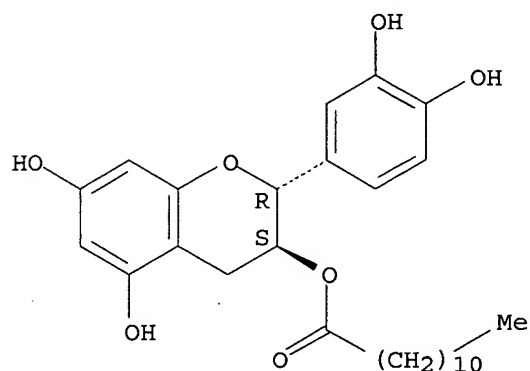
Absolute stereochemistry. Rotation (+).



RN 662144-62-9 HCAPLUS

CN Dodecanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

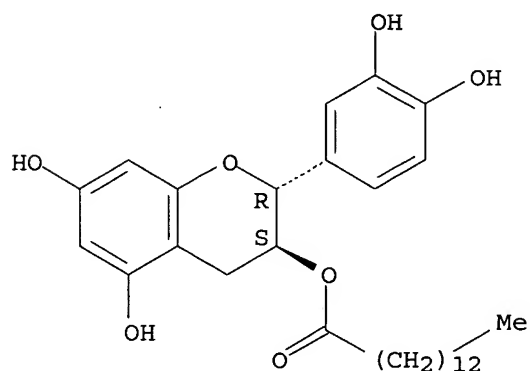
Absolute stereochemistry. Rotation (+).



RN 662144-63-0 HCAPLUS

CN Tetradecanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

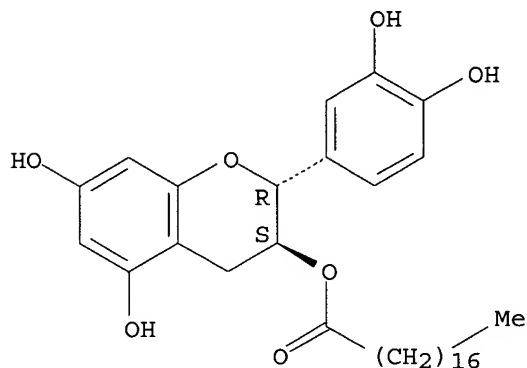
Absolute stereochemistry. Rotation (+).



RN 662144-64-1 HCAPLUS

CN Octadecanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 224433-78-7 299462-48-9 777953-04-5

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);

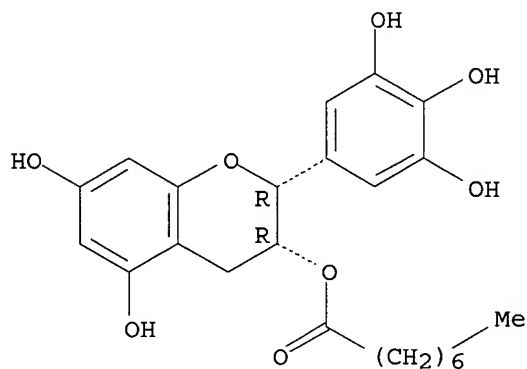
THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(bactericidal activity of; antimicrobial modified catechin compns. with increased lipophilicity)

RN 224433-78-7 HCAPLUS

CN Octanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

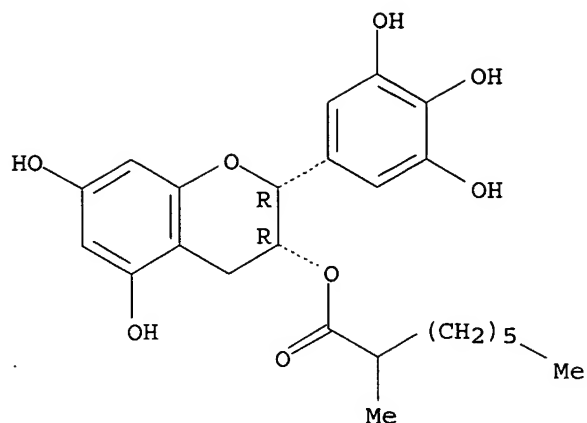
Absolute stereochemistry. Rotation (-).



RN 299462-48-9 HCAPLUS

CN Octanoic acid, 2-methyl-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

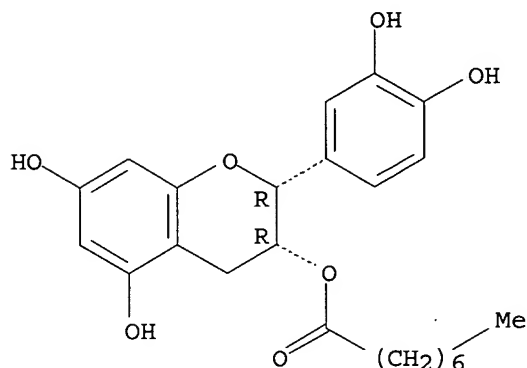
Absolute stereochemistry.



RN 777953-04-5 HCAPLUS

CN Octanoic acid, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 2 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:212389 HCAPLUS

DOCUMENT NUMBER: 142:285187

TITLE: Pollenosis-preventing tea leaf products containing antiallergic components

INVENTOR(S): Yamamoto, Mari; Nagai, Hiroshi

PATENT ASSIGNEE(S): National Institute of Agro-Environmental Sciences, Japan; Asahi Soft Drinks Co., Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005060277	A2	20050310	JP 2003-290789	20030808

PRIORITY APPLN. INFO.:

JP 2003-290789

20030808

AB The invention relates to a tea leaf product suitable for use in beverage, foods, gargles, nasal drops, eye washing solns., etc., for prevention of pollenosis, wherein the product contains antiallergic component, especially methylated catechin. obtained from specified variety of green tea leaves.

A tea bag containing green tea (Benifuji) leaves containing epigallocatechin-3-O-

(3-O-methyl)gallate 24.94 mg/bag was prepared, and applied to patients with Japanese cedar pollenosis.

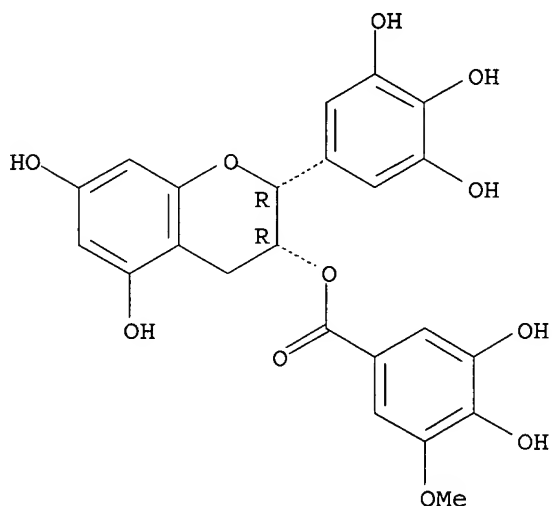
IT 83104-87-4 224434-07-5 676121-76-9
676121-77-0

RL: FFD (Food or feed use); NPO (Natural product occurrence); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses) (pollenosis-preventing tea leaf products containing antiallergic components)

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

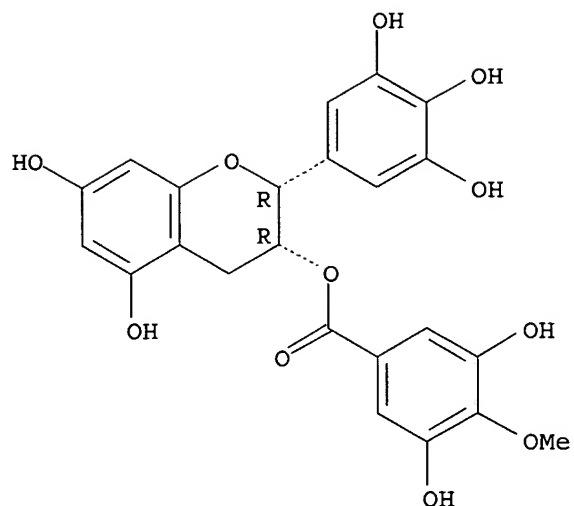
Absolute stereochemistry. Rotation (-).



RN 224434-07-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

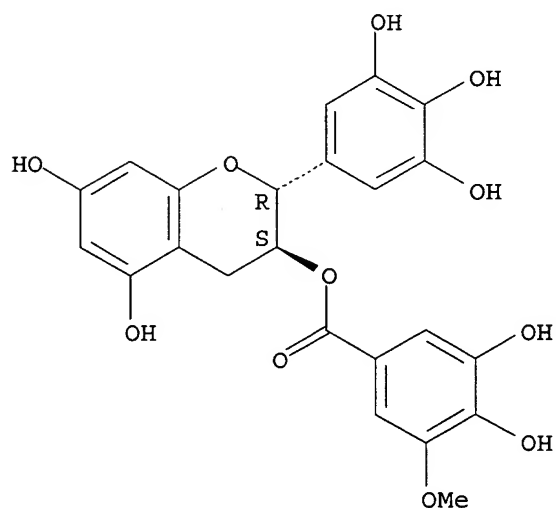
Absolute stereochemistry. Rotation (-).



RN 676121-76-9 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3S)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

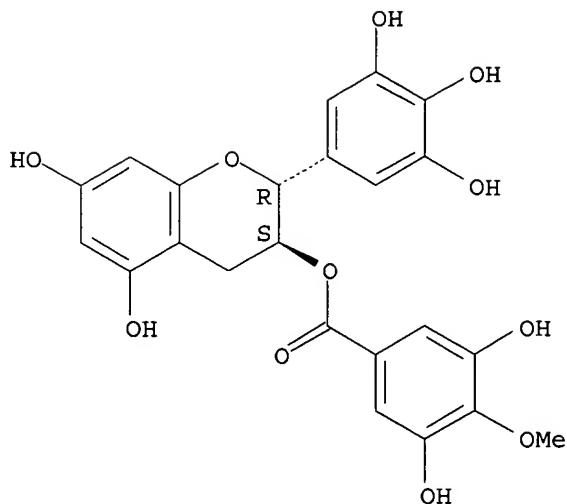
Absolute stereochemistry.



RN 676121-77-0 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3S)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 3 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:185391 HCAPLUS

DOCUMENT NUMBER: 142:261331

TITLE: Preparation of benzotropolone derivatives as
antioxidants and anti-inflammatory agents

INVENTOR(S): Ho, Chi-Tang; Ghai, Geetha; Sang, Shengmin; Jhoo,
Jin-Woo; Huang, Mou-Tuan; Rosen, Robert T.; Dushenkov,
Slavik

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 16 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005049284	A1	20050303	US 2003-652813	20030829
WO 2005021479	A1	20050310	WO 2004-US28164	20040830
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2003-652813 A 20030829

OTHER SOURCE(S): MARPAT 142:261331

AB The present invention discloses novel method of synthesizing benzotropolone compds., such as I [R1, R2, R3 = H, OH, alkoxy, alkyl, aryl, indolyl, Ph, benzyl, pyridinyl, pyrrolyl, thiophenyl], a salt or an ester of thereof, for their use as antioxidant and antiinflammatory agents. Thus, (-)-epicatechin and (-)-epigallocatechin were dissolved in

a mixture of acetone-pH 5.0 phosphate citrate buffer containing horseradish peroxidase, and treated with H₂O₂ to afford theaflavin (II). II exhibit relative oxygen-radical absorbance capacity (ORAC) value 11.60 ± 0.30 .

IT 220473-65-4P, Theaflavate B 691399-24-3P, Neotheaflavate B

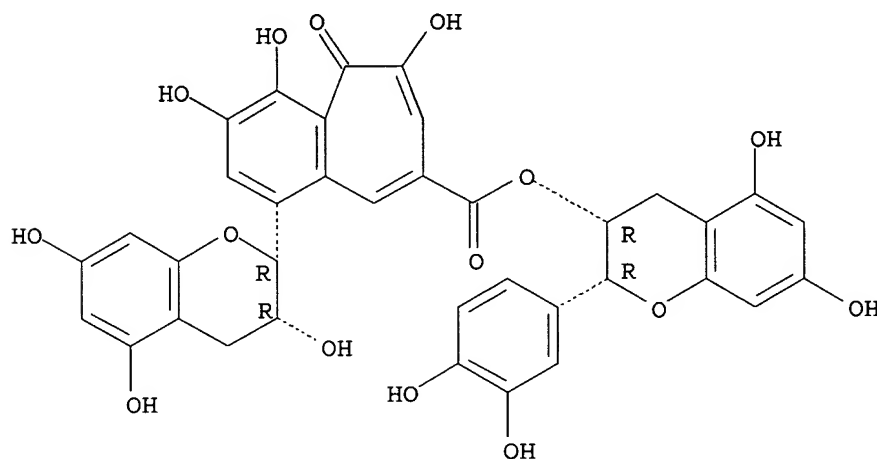
RL: BPN (Biosynthetic preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(enzymic synthesis of benzotropolone derivs. as antioxidants and antiinflammatory agents)

RN 220473-65-4 HCAPLUS

CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

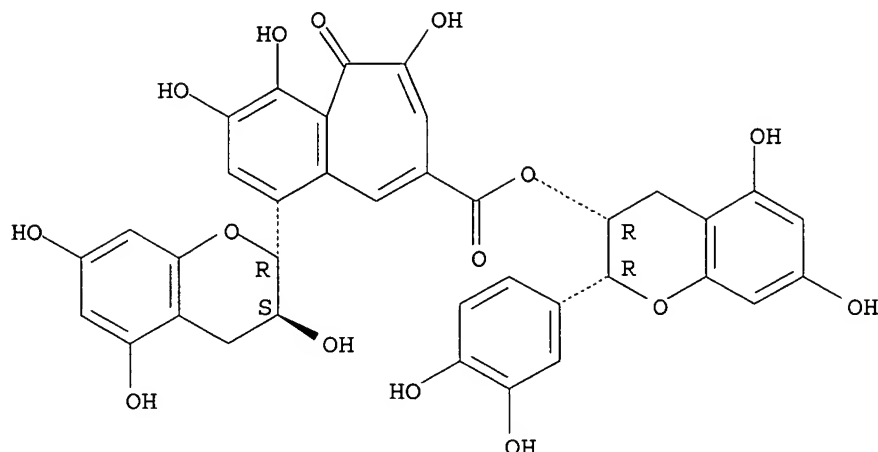
Absolute stereochemistry.



RN 691399-24-3 HCAPLUS

CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3S)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 4 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1035251 HCAPLUS
DOCUMENT NUMBER: 142:3076
TITLE: Development of catechin derivatives for preservation
of cells for transplantation and tissue regeneration
INVENTOR(S): Yagi, Kiyohito; Kawase, Masaya; Hara, Masahiko
PATENT ASSIGNEE(S): Mitsui Norin Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2004337110	A2	20041202	JP 2003-139728	20030519
PRIORITY APPLN. INFO.:			JP 2003-139728	20030519
OTHER SOURCE(S) :	MARPAT	142:3076		

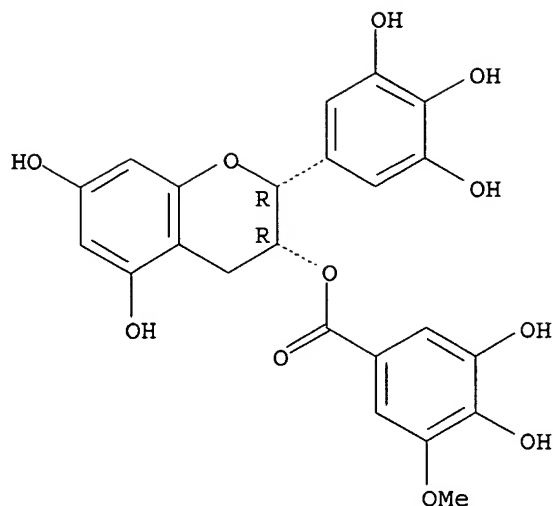
AB New protective substances for mammalian cells preservation has been developed. The substances are methylated catechins (I) (at least one of R1.apprx.R4 residues is methyl- and the others are hydrogen) and I with R3 = Me. The substances can be used for preservation of the animal cells that are useful in transplantation operations. The preservative effect of 3''-O-methyl-epigallocatechin gallate to maintain the viability of isolated rat hepatocytes was demonstrated.

IT 83104-87-4
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES
(Uses)
(cell protective material and protective method)

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L48 ANSWER 5 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:802565 HCAPLUS

DOCUMENT NUMBER: 141:314054

TITLE: Preparation of analogs of green tea polyphenols as chemotherapeutic and chemopreventive agents

INVENTOR(S): Zaveri, Nurulain; Chao, Wan-Ru; Bensari, Ahlem

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 33 pp., Cont.-in-part of U.S. Ser. No. 313,968.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004192723	A1	20040930	US 2003-731690	20031208
US 2004110790	A1	20040610	US 2002-313968	20021206
PRIORITY APPLN. INFO.:			US 2002-313968	A2 20021206

OTHER SOURCE(S): MARPAT 141:314054

AB Novel compds. useful as chemotherapeutic and chemopreventive agents are provided. The compds. are analogs of polyphenol catechins that occur in green tea, such as epigallocatechin-3-gallate (EGCG), and have the structure of formula I [R1-R3 = H, OH, alkyl, halo sulphydryl, alkoxy, aryloxy; R1R2, R2R3, R6R7, R8R9 may be linked to form a cyclic group; R4 = O, S, NH and CH2; R5 = SH, acyloxy, aroyloxy, NH2; R6-R9 = H, alkyl, alkoxy, aryloxy; R10, R11 = H, OH, alkyl, alkoxy, halo]. Pharmaceutical compns. are provided as well, as are methods of chemotherapy and chemoprevention. Thus, II (SR 13196) was prepared in several steps, and was found to have activity against breast cancer, lung tumor and colon adenocarcinoma cells.

IT 701284-11-9P, SR 13196 701284-12-0P, SR 13197

701284-14-2P, SR 13200 701284-17-5P, SR 13913

765956-07-8P, SR 13916 765956-22-7P, SR 13920

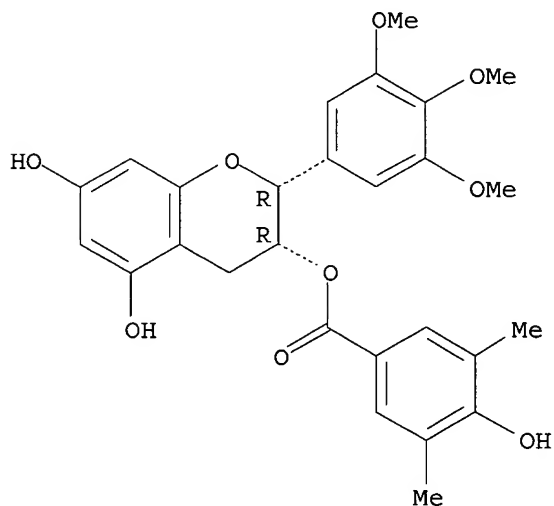
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of polyphenol catechins as chemotherapeutic and chemopreventive agents)

RN 701284-11-9 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethyl-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trimethoxyphenyl)-2H-1-benzopyran-3-yl ester, rel- (9CI) (CA INDEX NAME)

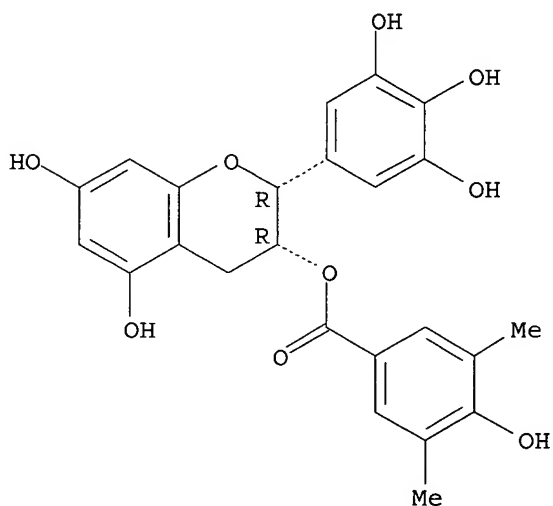
Relative stereochemistry.



RN 701284-12-0 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethyl-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

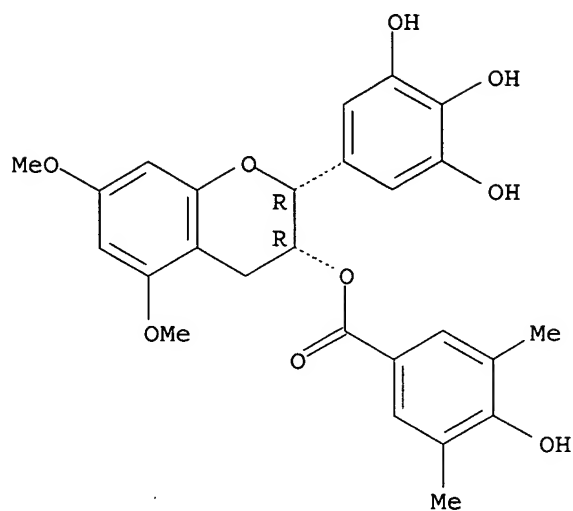


RN 701284-14-2 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethyl-, (2R,3R)-3,4-dihydro-5,7-dimethoxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, rel- (9CI) (CA INDEX NAME)

NAME)

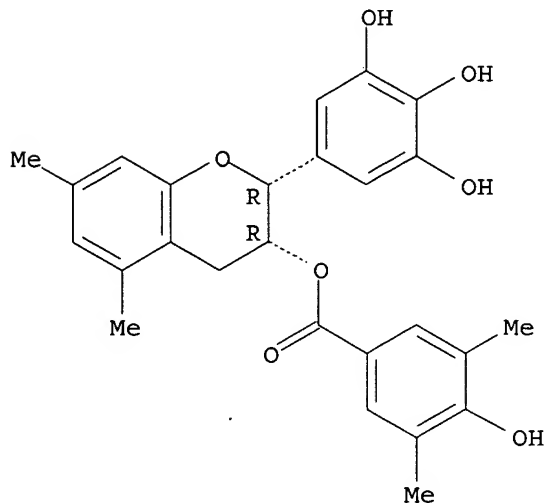
Relative stereochemistry.



RN 701284-17-5 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethyl-, (2R,3R)-3,4-dihydro-5,7-dimethyl-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, rel- (9CI) (CA INDEX NAME)

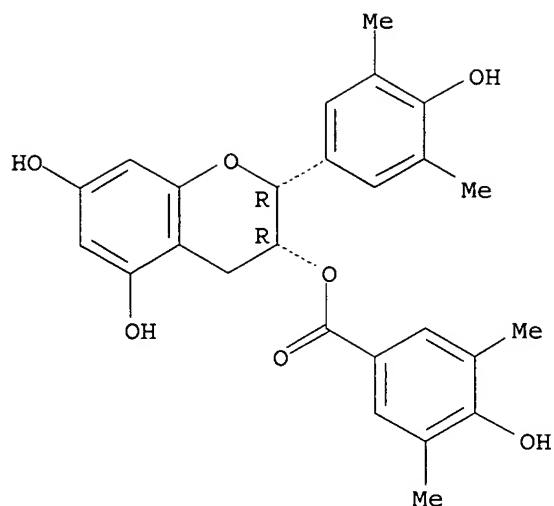
Relative stereochemistry.



RN 765956-07-8 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethyl-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(4-hydroxy-3,5-dimethylphenyl)-2H-1-benzopyran-3-yl ester, rel- (9CI) (CA INDEX NAME)

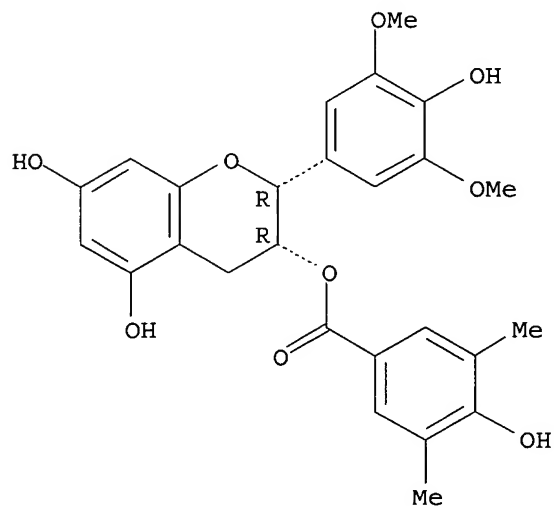
Relative stereochemistry.



RN 765956-22-7 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethyl-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-2H-1-benzopyran-3-yl ester, rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



L48 ANSWER 6 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:722920 HCAPLUS

DOCUMENT NUMBER: 141:230734

TITLE: Alpha-glucosidase inhibitors and their synthesis from a natural source

INVENTOR(S): Rao, Janaswamy Madhusudana; Rao, Rao Jagadeeshwar; Kumar, Upparapalli Sampath; Reddy, Singireddy Venkat; Tiwari, Ashok Kumar; Yadav, Jhillusingh; Raghavan, Kondapuram Vijaya

PATENT ASSIGNEE(S): Council of Scientific & Industrial Research, India

SOURCE: U.S. Pat. Appl. Publ., 9 pp., Cont.-in-part of U.S.

Ser. No. 375,033.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004171674	A1	20040902	US 2003-403034	20030401
US 2004116716	A1	20040617	US 2003-375033	20030228
US 6781002	B2	20040824		
PRIORITY APPLN. INFO.:			US 2003-375033	A2 20030228
			WO 2002-IB5426	A1 20021217

OTHER SOURCE(S): MARPAT 141:230734

AB The present invention provides novel α -glucosidase inhibitory compound (-)-mesquitol and its analogs isolated in significant yield from traditional medicinal plant *Dichrostachys cinerea* and further modification of (-)-mesquitol to enhance the α -glucosidase inhibitory potential; the invention also identifies the usage of (-)-mesquitol and its analogs, based on their α -glucosidase inhibitory activity, as broad based potential therapeutics as antihyperglycemic, antidiabetic, antiobesity, antiviral, anticancer, immunostimulants and the like.

IT 609337-48-6P 609337-49-7P 609337-50-0P
 609337-51-1P 609337-52-2P 609337-53-3P
 609337-54-4P 609337-55-5P 609337-56-6P
 609337-57-7P 609337-58-8P

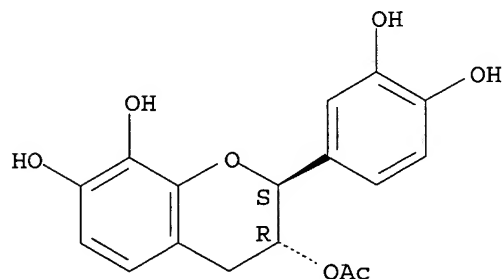
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(α -glucosidase inhibitors and their synthesis from (-)-mesquitol isolated from *Dichrostachys cinerea*)

RN 609337-48-6 HCAPLUS

CN 2H-1-Benzopyran-3,7,8-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, 3-acetate, (2S,3R)- (9CI) (CA INDEX NAME)

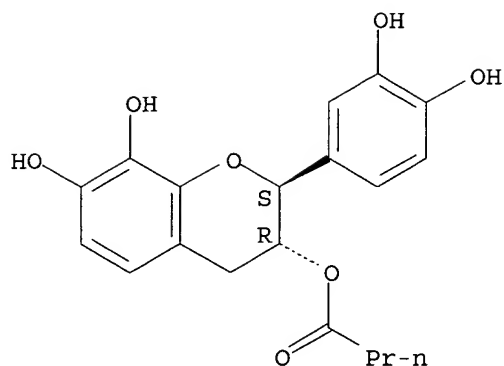
Absolute stereochemistry.



RN 609337-49-7 HCAPLUS

CN Butanoic acid, (2S,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-7,8-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

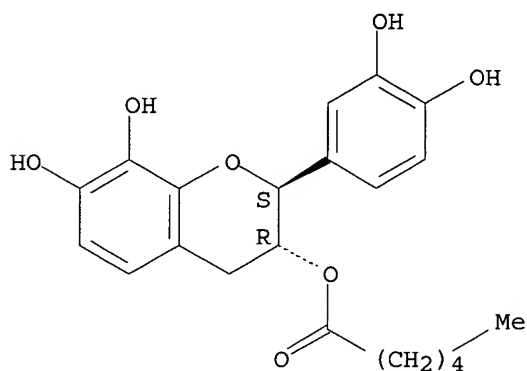
Absolute stereochemistry.



RN 609337-50-0 HCAPLUS

CN Hexanoic acid, (2S,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-7,8-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

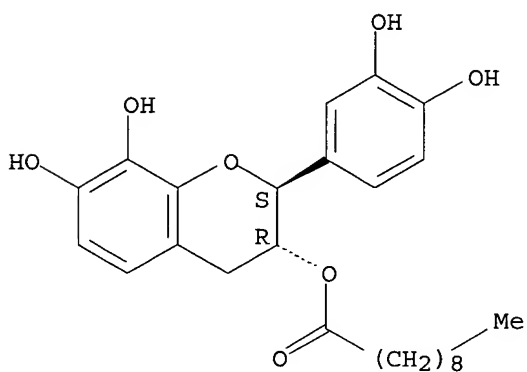
Absolute stereochemistry.



RN 609337-51-1 HCAPLUS

CN Decanoic acid, (2S,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-7,8-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

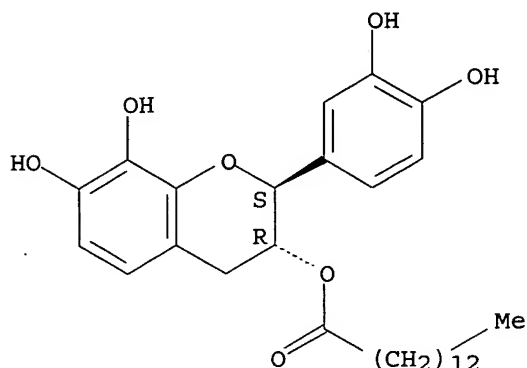


RN 609337-52-2 HCAPLUS

CN Tetradecanoic acid, (2S,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-7,8-

dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

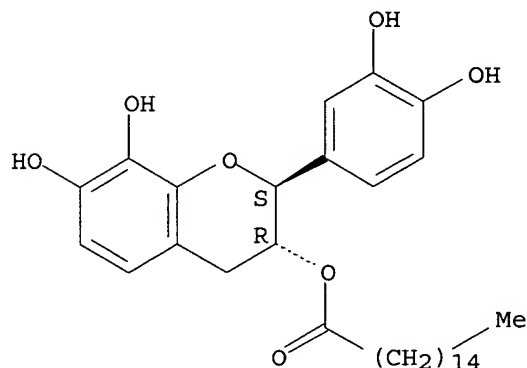
Absolute stereochemistry.



RN 609337-53-3 HCAPLUS

CN Hexadecanoic acid, (2S,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-7,8-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

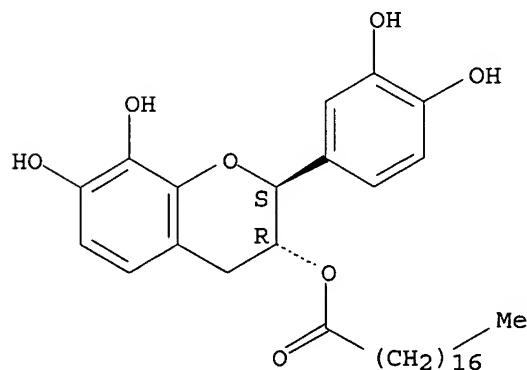
Absolute stereochemistry.



RN 609337-54-4 HCAPLUS

CN Octadecanoic acid, (2S,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-7,8-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

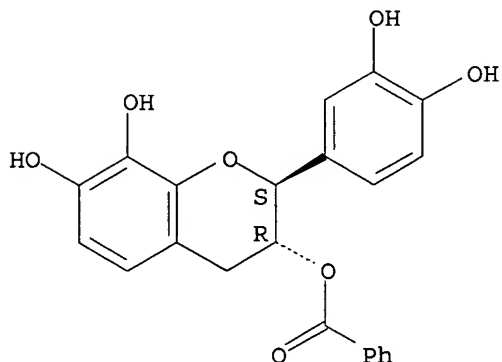
Absolute stereochemistry.



RN 609337-55-5 HCAPLUS

CN 2H-1-Benzopyran-3,7,8-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-,
3-benzoate, (2S,3R)- (9CI) (CA INDEX NAME)

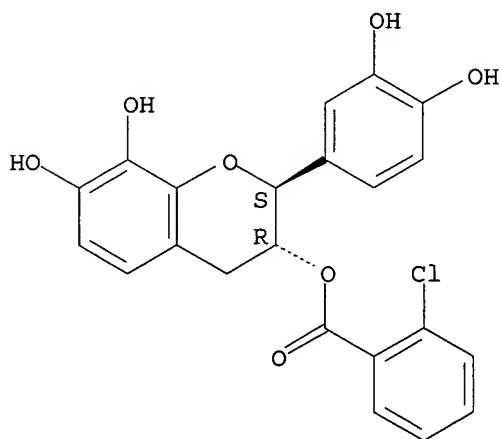
Absolute stereochemistry.



RN 609337-56-6 HCAPLUS

CN Benzoic acid, 2-chloro-, (2S,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-7,8-
dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

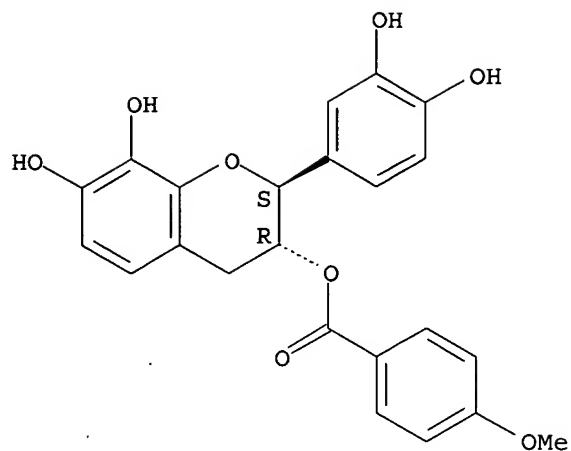
Absolute stereochemistry.



RN 609337-57-7 HCAPLUS

CN Benzoic acid, 4-methoxy-, (2S,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-7,8-
dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

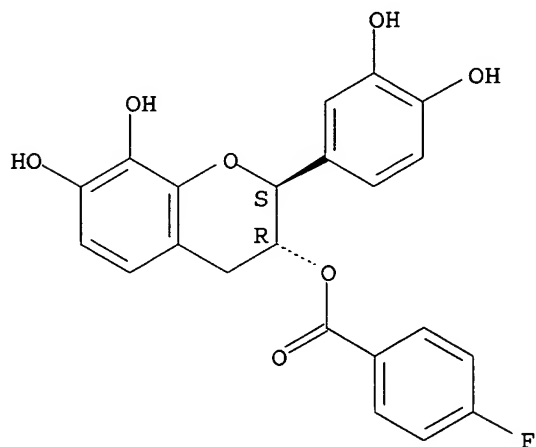
Absolute stereochemistry.



RN 609337-58-8 HCAPLUS

CN Benzoic acid, 4-fluoro-, (2S,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-7,8-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 7 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:649414 HCAPLUS

DOCUMENT NUMBER: 141:173382

TITLE: Antiallergy functional foods and beverages,
antiallergy tea leaves, and enhancement of antiallergy
activity of the tea leaves and the functional foods

INVENTOR(S): Yamamoto, Mari; Nagai, Hiroshi

PATENT ASSIGNEE(S): Bio-Oriented Technology Research Advancement Institute
Brai-Jp, Japan; National Institute of
Agro-Environmental Sciences; Asahi Soft Drinks Co.,
Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004222683	A2	20040812	JP 2003-18019	20030127
JP 2005185292	A2	20050714	JP 2005-57288	20050302
PRIORITY APPLN. INFO.:			JP 2003-18019	A3 20030127

AB The antiallergy activity of tea leaves containing antiallergy components are enhanced by extraction at 50-100° to increase extraction efficiencies and isomerization of catechins. Antiallergy food materials rich in epigallocatechin 3-O-(3-O-methyl)gallate, epigallocatechin 3-O-(4-O-methyl)gallate, and/or their isomers are obtained. The antiallergy activity of functional foods containing the tea leaves containing antiallergy components are enhanced by heat-sterilization and extraction at 50-100°.

IT 83104-87-4 224434-07-5

RL: FFD (Food or feed use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

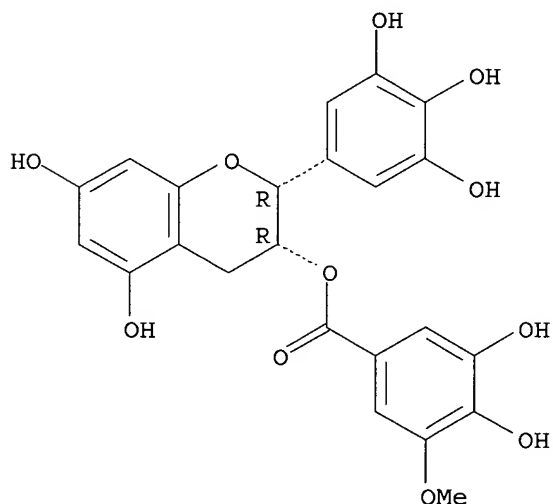
(enhancement of antiallergy activity of tea leaves and functional foods by high-temperature extraction and sterilization to increase extraction efficiencies

and isomerization of catechins)

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

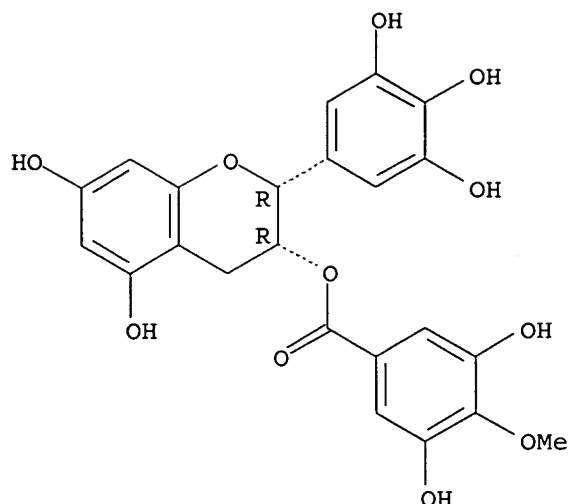
Absolute stereochemistry. Rotation (-).



RN 224434-07-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L48 ANSWER 8 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:649413 HCAPLUS

DOCUMENT NUMBER: 141:173381

TITLE: Removal of caffeine from tea leaves containing antiallergy components, antiallergy tea leaf products, their manufacture, their use for functional foods and beverages, and tea bags

INVENTOR(S): Yamamoto, Mari; Nagai, Hiroshi

PATENT ASSIGNEE(S): Bio-Oriented Technology Research Advancement Institute
Brai-Jp, Japan; National Institute of
Agro-Environmental Sciences; Asahi Soft Drinks Co.,
Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004222682	A2	20040812	JP 2003-18018	20030127
JP 3706875	B2	20051019		

PRIORITY APPLN. INFO.: JP 2003-18018 20030127

AB Fresh tea leaves containing antiallergy components are immersed in hot water at 85-95° for 30 s to 2 min, dewatered for caffeine removal, and steamed to give crude tea products. The tea products contain epigallocatechin 3-O-(3-O-methyl)gallate, epigallocatechin 3-O-(4-O-methyl)gallate, and/or strictinin as antiallergy components. The exts. or powders of the tea leaf products are useful for functional foods and beverages.

IT 83104-87-4 224434-07-5

RL: FFD (Food or feed use); PAC (Pharmacological activity); THU

(Therapeutic use); BIOL (Biological study); USES (Uses)

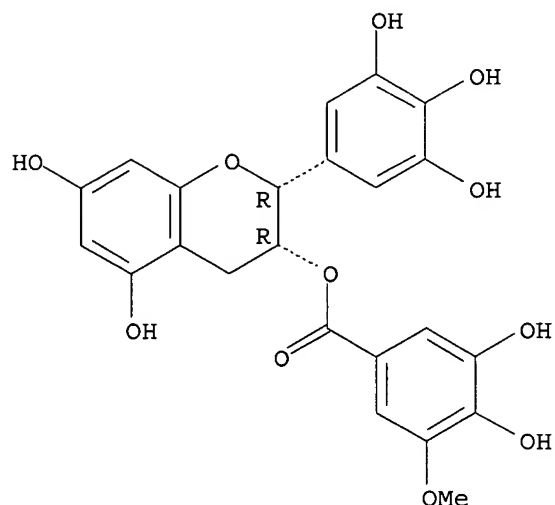
(removal of caffeine from tea leaves for antiallergy tea leaf products and functional foods and beverages)

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-

2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

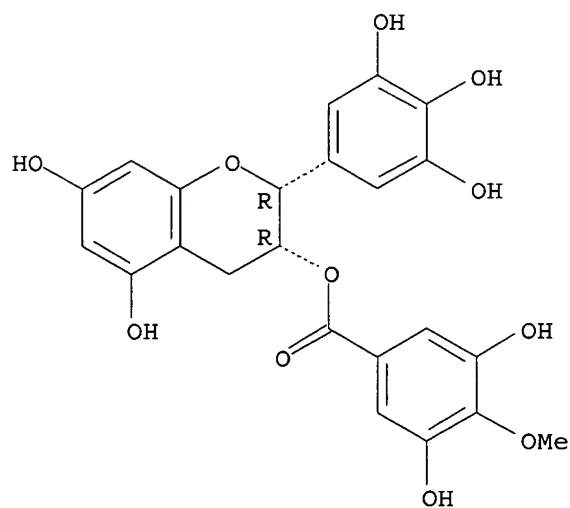
Absolute stereochemistry. Rotation (-).



RN 224434-07-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L48 ANSWER 9 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:647648 HCAPLUS

DOCUMENT NUMBER: 141:173379

TITLE: Tea leaves having antiallergy activity, their use for functional foods, and control of the ratios of epigallocatechin methylgallates to strictinin in the

tea leaves and functional foods
 INVENTOR(S): Yamamoto, Mari; Nagai, Hiroshi
 PATENT ASSIGNEE(S): Bio-Oriented Technology Research Advancement Institute
 Brai-Jp, Japan; National Institute of
 Agro-Environmental Sciences; Asahi Soft Drinks Co.,
 Ltd.
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: **Patent**
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004222681	A2	20040812	JP 2003-18017	20030127
PRIORITY APPLN. INFO.:			JP 2003-18017	20030127

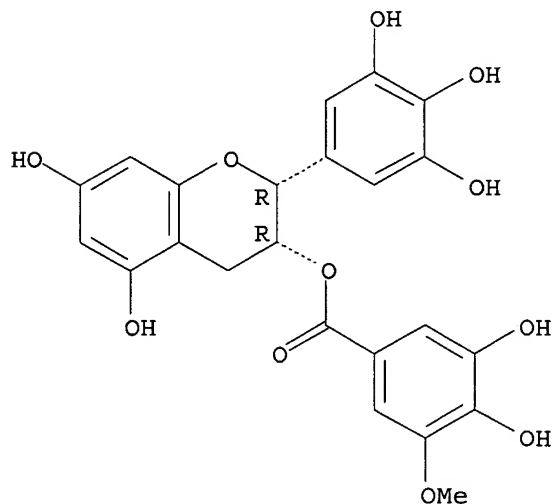
AB The tea leaves contain antiallergy components and have woody stem content ≤5 weight%. The ratios of epigallocatechin 3-O-(3-O-methyl)gallate and epigallocatechin 3-O-(4-O-methyl)gallate to strictinin are controlled by selecting the leaf positions and the degree of maturity of the tea leaves.

IT **83104-87-4 224434-07-5**
 RL: FFD (Food or feed use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (tea leaves containing antiallergy components, epigallocatechin methylgallates and strictinin, for functional foods)

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

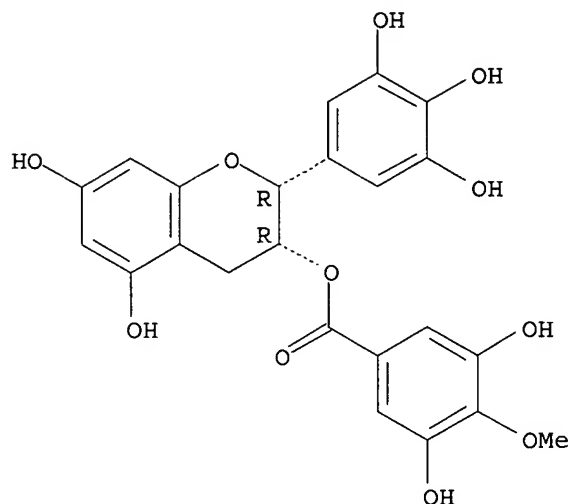
Absolute stereochemistry. Rotation (-).



RN 224434-07-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L48 ANSWER 10 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:473358 HCAPLUS

DOCUMENT NUMBER: 141:38529

TITLE: Preparation of catechin benzoyl esters as anticancer agents.

INVENTOR(S): Zaveri, Nurulain; Chao, Wan-Ru; Bensari, Ahlem

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 27 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004110790	A1	20040610	US 2002-313968	20021206
CA 2508020	AA	20040624	CA 2003-2508020	20031208
WO 2004052873	A2	20040624	WO 2003-US39191	20031208
WO 2004052873	C2	20040812		
WO 2004052873	A3	20050106		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004192723	A1	20040930	US 2003-731690	20031208
EP 1581512	A2	20051005	EP 2003-796871	20031208
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:			US 2002-313968	A 20021206

WO 2003-US39191

W 20031208

OTHER SOURCE(S): MARPAT 141:38529

AB Title compds. I [R1, R2, R3 = OH, halo, SH, etc.; R4 = O, S, NRx, etc.; Rx = H, alkyl; R5 = OH, SH, acyloxy, etc.; R6, R7, R8, R9 = H, alkyl, alkoxy, etc.; R10, R11 = H, OH, alkyl, etc.] and their pharmaceutically acceptable salts were prepared. For example, O-acylation of catechin II, e.g., prepared from 2',4',6'-trihydroxyacetophenone in 6-steps, with 3,5-dimethyl-4-(phenylmethoxy)benzoic acid followed by benzyl ether hydrogenation, afforded catechin II. In MCF-7 (ER+) breast cancer cell line inhibition growth assays, 3-examples of compds. I exhibited IC50 values ranging from 11.05->100 μ M, e.g., the IC50 value of catechin III was 11.05 μ M. Of note, compds. I are analogs of polyphenol catechins that occur in green tea. Compds. I are claimed useful as chemotherapeutic and chemopreventive agents.

IT 701284-11-9P 701284-12-0P 701284-14-2P

701284-17-5P

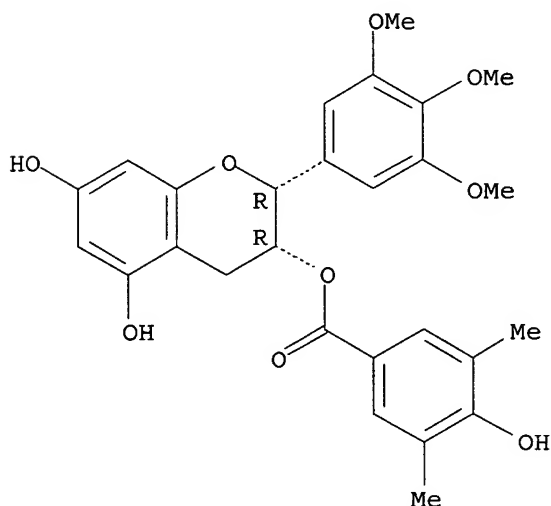
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of catechin benzoyl esters as anticancer agents.)

RN 701284-11-9 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethyl-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trimethoxyphenyl)-2H-1-benzopyran-3-yl ester, rel- (9CI) (CA INDEX NAME)

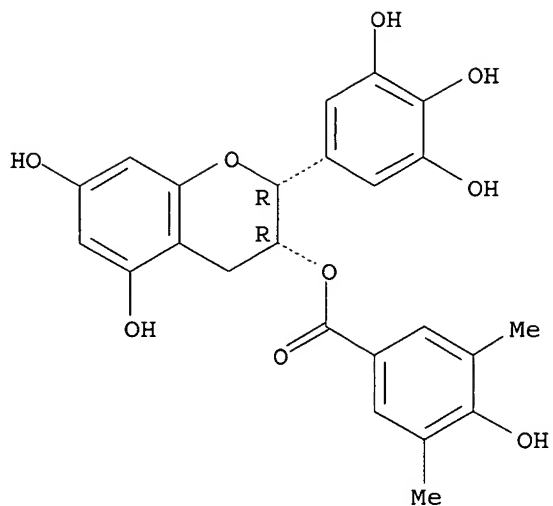
Relative stereochemistry.



RN 701284-12-0 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethyl-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, rel- (9CI) (CA INDEX NAME)

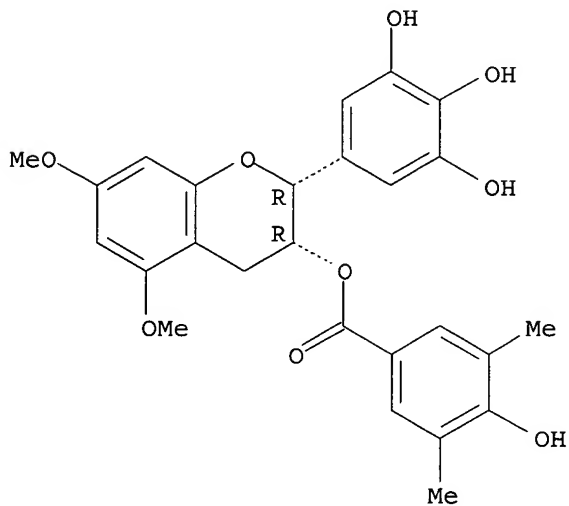
Relative stereochemistry.



RN 701284-14-2 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethyl-, (2R,3R)-3,4-dihydro-5,7-dimethoxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, rel- (9CI) (CA INDEX NAME)

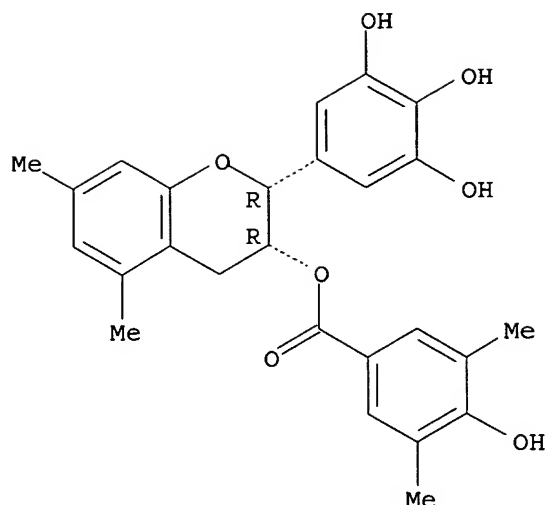
Relative stereochemistry.



RN 701284-17-5 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethyl-, (2R,3R)-3,4-dihydro-5,7-dimethyl-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L48 ANSWER 11 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:264814 HCAPLUS

DOCUMENT NUMBER: 140:286534

TITLE: Functional foods/drinks containing antiallergic component

INVENTOR(S): Kitani, Seiichi; Nagai, Hiroshi; Hashizume, Shuichi; Sato, Susumu; Yamamoto, Mari

PATENT ASSIGNEE(S): Asahi Soft Drinks Co., Ltd., Japan; Morinaga & Co., Ltd.; Independent Administrative Institute, National Agricultural Research Organization

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026047	A1	20040401	WO 2003-JP11775	20030916
W: CN, KR, US				
RW: CH, DE, FR, GB, NL				
JP 2004105078	A2	20040408	JP 2002-271730	20020918
EP 1547474	A1	20050629	EP 2003-797612	20030916
R: CH, DE, FR, GB, LI, NL				

PRIORITY APPLN. INFO.:				
	JP 2002-271730	A	20020918	
	WO 2003-JP11775	W	20030916	

AB A functional food/drink contains ≥ 1 compound selected from the group consisting of epigallocatechin-3-O-(3-O-methyl)gallate, gallocatechin-3-O-(3-O-methyl)gallate, epigallocatechin-4-O-(4-O-methyl)gallate, gallocatechin-4-O-(4-O-methyl)gallate and strychnine. These compds. are derived from Chinese tea.

IT 83104-87-4 224434-07-5 676121-76-9
676121-77-0

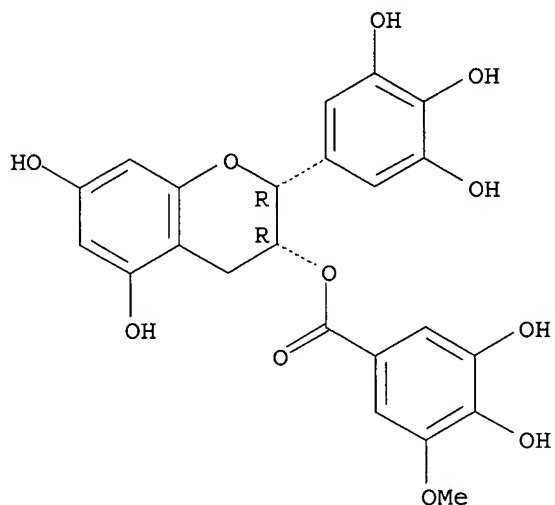
RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(as anti-allergy compound for health food)

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-

2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

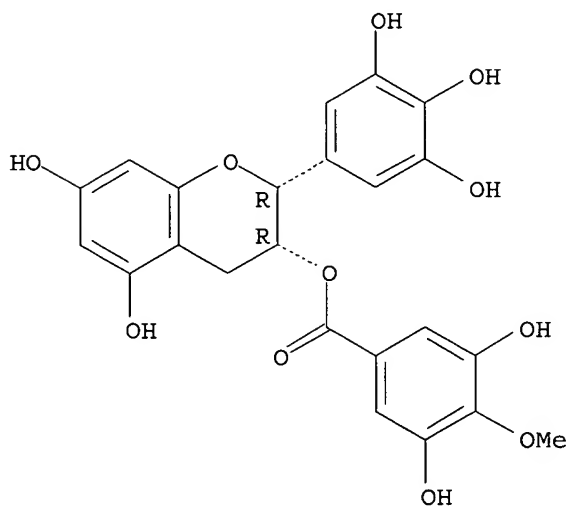
Absolute stereochemistry. Rotation (-).



RN 224434-07-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

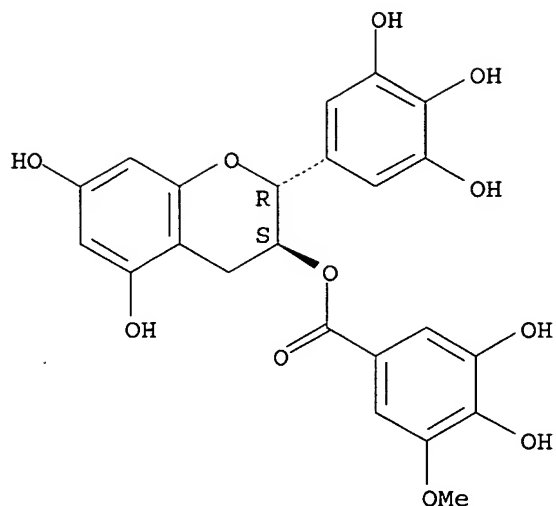
Absolute stereochemistry. Rotation (-).



RN 676121-76-9 HCAPLUS

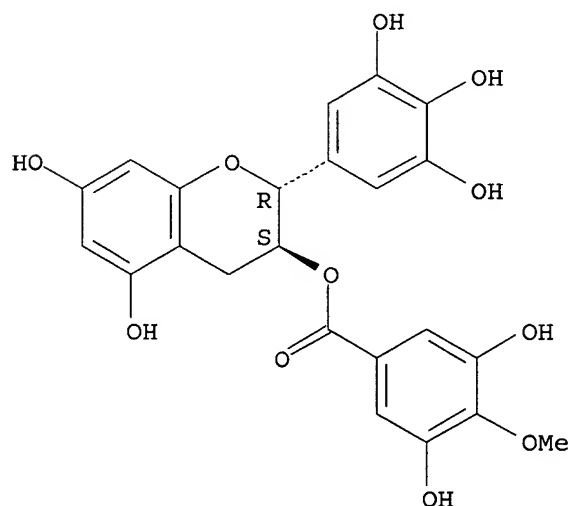
CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3S)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 676121-77-0 HCAPLUS
CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3S)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 12 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:652131 HCAPLUS
DOCUMENT NUMBER: 139:214237
TITLE: Preparation of nitrate prodrugs able to release nitric oxide in a controlled and selective way and their use for prevention and treatment of inflammatory, ischemic and proliferative diseases
INVENTOR(S): Scaramuzzino, Giovanni
PATENT ASSIGNEE(S): Italy

SOURCE: Eur. Pat. Appl., 313 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1336602	A1	20030820	EP 2002-425075	20020213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.: EP 2002-425075 20020213

AB New pharmaceutical compds. of general formula F-(X)_q (I) [q = 1-5, preferably 1; F is chosen among drugs such as δ -tocopherol, clidanac, diethylhomospermine, glucosamine, thymocartin, vofopitant, etc.; X is chosen among 4 groups M, T, V, and Y where M = ONO₂, nitrate salt, nitrite ester, ONO, thionitrite, SNO, etc., T = OR₁-M, OR₁OR₁-M, SR₁NR₂R₁-M, NR₂R₁-M, NR₂R₁SR₁-M, etc., R₁ = saturated or unsatd., linear or branched alkylene, having 1 to 21 carbon atoms or a saturated or unsatd., optionally heterosubstituted or branched cycloalkylene, having 3 to 7 carbon atoms or an optionally heterosubstituted arylene having 3 to 7 carbon atoms; R₂ = H, saturated or unsatd., linear or branched 1-21 carbon atom alkyl, saturated or unsatd. optionally heterosubstituted or branched 3-7 carbon cycloalkyl, optionally heterosubstituted 3-7 carbon aryl; R₁, R₂ = OH, SH, F, Cl, Br, OPO₃H₂, CO₂H, etc.; bond between F and T = carboxylic ester, carboxylic amide, glycoside, azo, thioester, sulfonic ester, etc.; V = Z-M₂, OZ-M₂, NR₂Z-M₂, R₁Z-M₂, OR₁-M₂, OR₁Z-M₂, M₂ = M, R₁-M, OR₁-M, SR₁-M, NR₂R₁-M; ZM₂ = COCH₂CH(M₂)CH₂N+Me₃, COCH₂CH₂COM₂, COCH(NHR₂)CH₂M₂, etc.; Y = 4-COC₆H₄CH₂ONO₂, O(CH₂)₄ONO₂, COCH(NH₂)CH₂ONO₂, 3-OC₆H₄CH₂ONO₂, etc.] were prepared For example, α -tocopherol reacted with 4-HO₂CC₆H₄CH₂ONO₂ to give the nitroxymethyl derivative II. The compds. of general formula I are nitrate prodrugs which can release nitric oxide in vivo in a controlled and selective way and without hypotensive side effects and for this reason they are useful for the preparation of medicines for prevention and treatment of inflammatory, ischemic, degenerative and proliferative diseases of musculoskeletal, tegumental, respiratory, gastrointestinal, genito-urinary and central nervous systems.

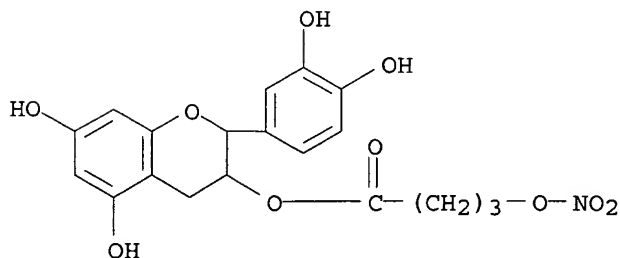
IT 586350-55-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitrate prodrugs for treating or preventing inflammatory, ischemic, degenerative, and proliferative diseases)

RN 586350-55-2 HCAPLUS

CN Butanoic acid, 4-(nitrooxy)-, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 13 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:633887 HCAPLUS

DOCUMENT NUMBER: 139:176980

TITLE: MICAL proteins of Drosophila and human interacting with CAS-L protein and playing a role in axonal repulsion and their uses

INVENTOR(S): Kolodkin, Alex L.; Terman, Jon Richard; Mao, Tianyi; Pasterkamp, Ronald Jeroen; Yu, Hung-hsiang

PATENT ASSIGNEE(S): The Johns Hopkins University School of Medicine, USA

SOURCE: PCT Int. Appl., 367 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

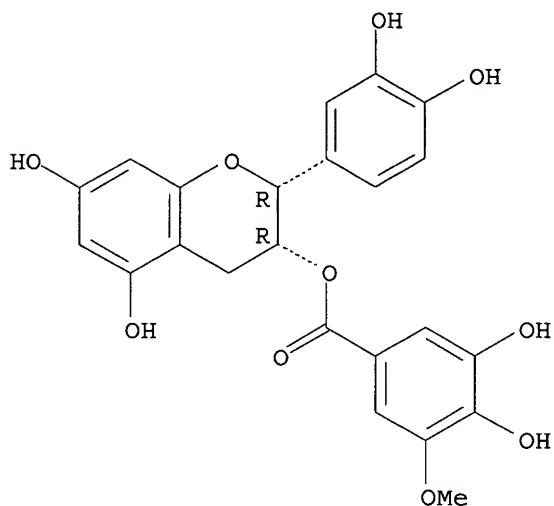
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003066821	A2	20030814	WO 2003-US3551	20030204
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2003232419	A1	20031218	US 2003-359012	20030204
EP 1572907	A2	20050914	EP 2003-713377	20030204
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
PRIORITY APPLN. INFO.:			US 2002-354178P	P 20020204
			US 2002-384302P	P 20020530
			US 2002-388325P	P 20020613
			WO 2003-US3551	W 20030204
AB	Proteins that interact with CAS-L Cas-L (Crk-associated substrate-related protein, lymphocyte) and that play a role in plexin-mediated axonal repulsion are identified in Drosophila and human and genes encoding them are cloned. The proteins (MICAL: mol. interacting with CAS-L) and genes may be used in identifying agents that affect axon growth and placement. Furthermore, provided herein are methods for affecting axon growth and placement. The proteins were first identified in a two-hybrid screen for proteins interacting with Drosophila plexin A. The mRNA is widely distributed in the Drosophila embryo. P-element inactivation of the gene gave rise to flies with deficiencies in axonal guidance comparable to those seen in mutations in genes for semaphorins and plexins. The protein has a functional flavin monooxygenase domain that is essential for interactions with semaphorins. Gallic acid derivs. blocked semaphorin 3A axonal repulsion.			
IT	83104-86-3 83104-87-4 264147-80-0			
RL:	BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)			
	(as inhibitor of flavin monooxygenase and axonal repulsion; MICAL proteins of Drosophila and human interacting with CAS-L protein and			

playing role in axonal repulsion and their uses)

RN 83104-86-3 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

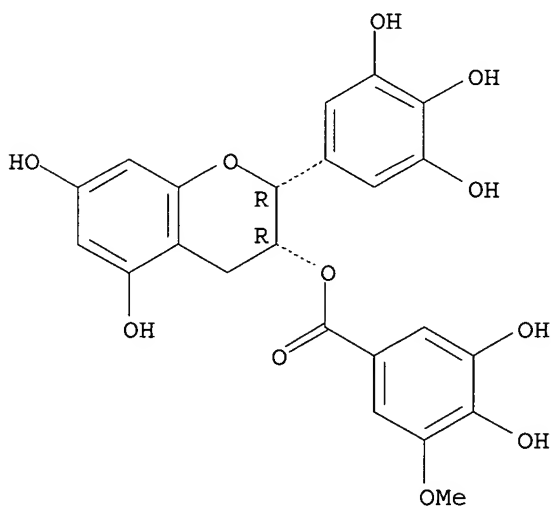
Absolute stereochemistry. Rotation (-).



RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

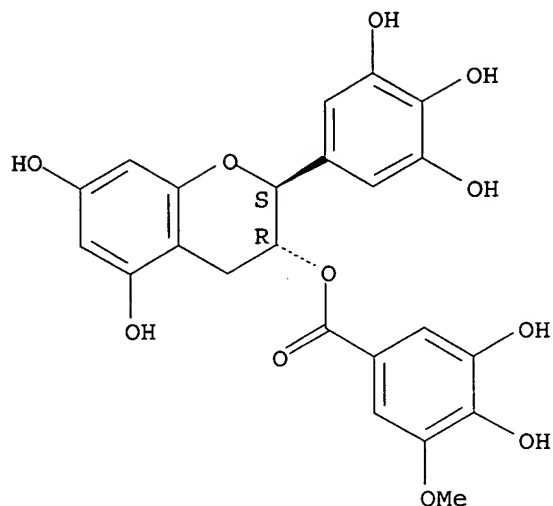
Absolute stereochemistry. Rotation (-).



RN 264147-80-0 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2S,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L48 ANSWER 14 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:435300 HCAPLUS

DOCUMENT NUMBER: 138:406983

TITLE: Method and compositions for regulation of 5- α -reductase activity

INVENTOR(S): Liao, Shutsung; Hiipakka, Richard

PATENT ASSIGNEE(S): University of Chicago Office of Technology and Intellectual Property, USA

SOURCE: U.S. Pat. Appl. Publ., 44 pp., Cont.-in-part of U.S. Ser. No. 530,443.

CODEN: USXXCO

DOCUMENT TYPE: **Patent**

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 8

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003105030	A1	20030605	US 2002-132050	20020424
US 6696484	B2	20040224		
WO 9922728	A1	19990514	WO 1998-US23041	19981030
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6576660	B1	20030610	US 2000-530443	20000428
PRIORITY APPLN. INFO.:			US 1997-63770P	P 19971031
			WO 1998-US23041	W 19981030
			US 2000-530443	A2 20000428
AB Pharmaceutical compns. and methods for treating androgen-related disorders are disclosed. The pharmaceutical compns. may include a				

5- α -reductase inhibitor, such as natural and synthetic flavanoids, catechols, curcumin-related substances, quinones, catechins, particularly epigallocatechin derivs., fatty acids, and the salts, esters, analogs, pro-drugs, isomers, racemic mixts., or derivs. of any of the foregoing. The use of testosterone (or DHT) combinations with the aforementioned 5- α -reductase inhibitor compds. is also contemplated.

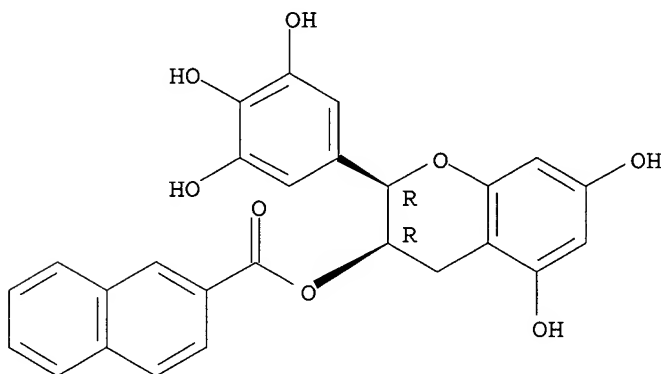
IT 224433-76-5, HZIV 120

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(HZIV 120; method and compns. for regulation of 5- α -reductase activity)

RN 224433-76-5 HCAPLUS

CN 2-Naphthalenecarboxylic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 224441-46-7, HZIV 134

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(HZIV 134; method and compns. for regulation of 5- α -reductase activity)

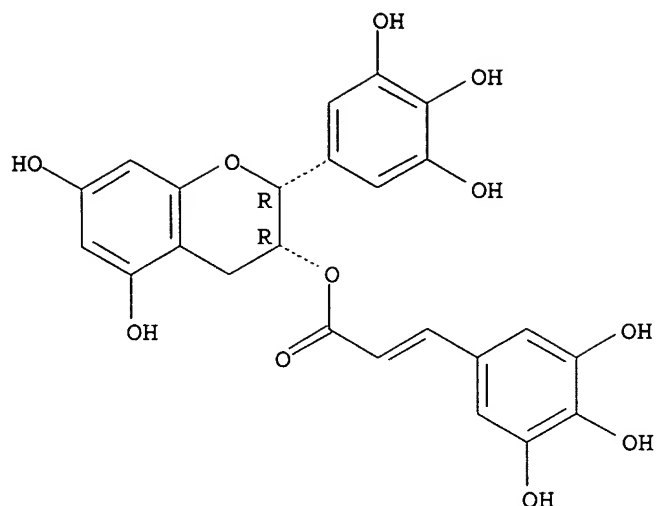
RN 224441-46-7 HCAPLUS

CN 2-Propenoic acid, 3-(3,4,5-trihydroxyphenyl)-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

Currently available stereo shown.



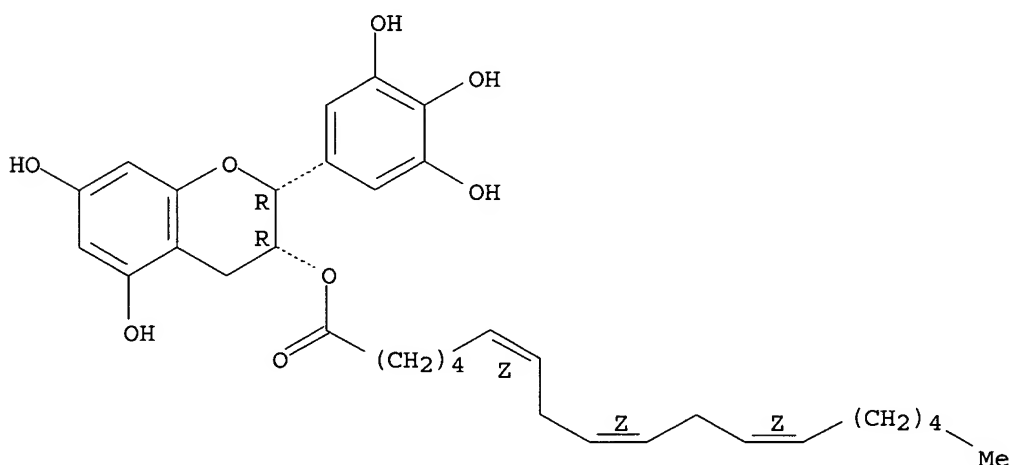
IT 224441-50-3, HZIV 142

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(HZIV 142; method and comps. for regulation of 5- α -reductase activity)

RN 224441-50-3 HCAPLUS

CN 6,9,12-Octadecatrienoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, (6Z,9Z,12Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



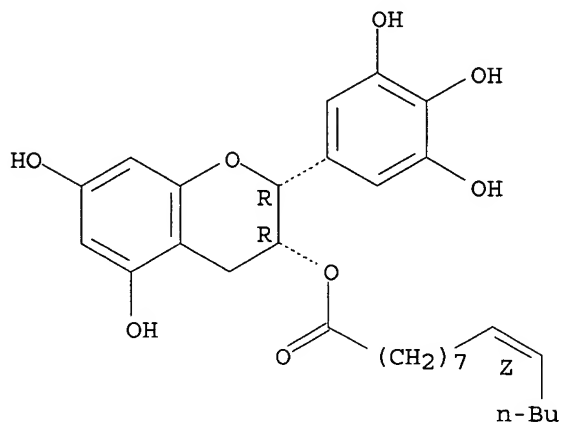
IT 224441-44-5, HZIV 160

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(HZIV 160; method and comps. for regulation of 5- α -reductase activity)

RN 224441-44-5 HCAPLUS

CN 9-Tetradecenoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, (9Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



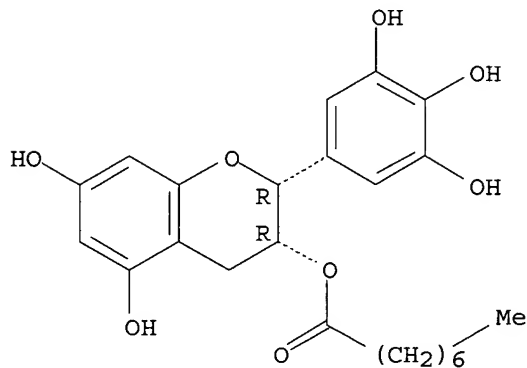
IT 224433-78-7, HZIV 166

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(HZIV 166; method and compns. for regulation of 5- α -reductase activity)

RN 224433-78-7 HCAPLUS

CN Octanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



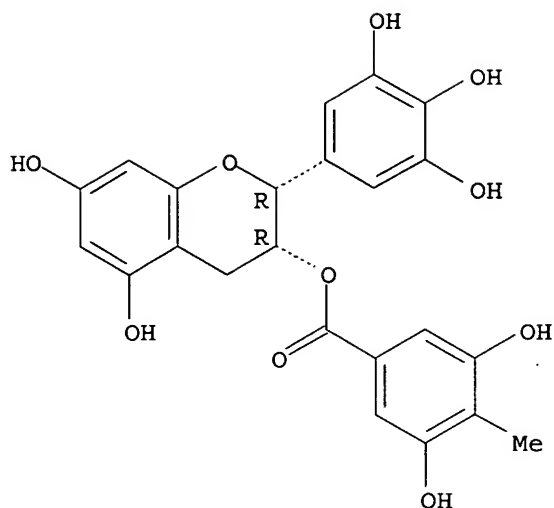
IT 224441-52-5, HZIV 68

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(HZIV 68; method and compns. for regulation of 5- α -reductase activity)

RN 224441-52-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methyl-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



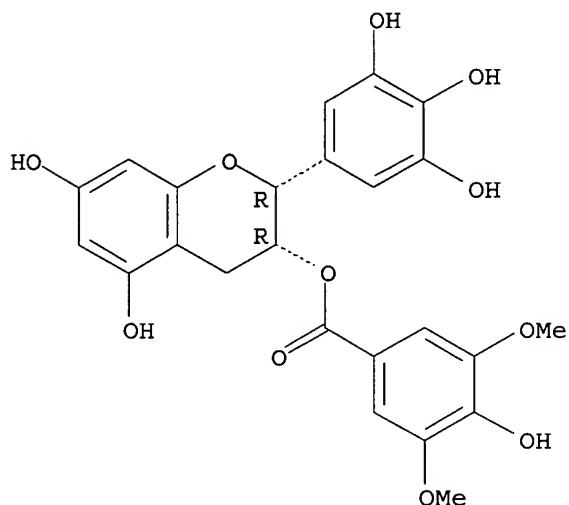
IT 173484-92-9, HZIV 75

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(HZIV 75; method and compns. for regulation of 5- α -reductase activity)

RN 173484-92-9 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



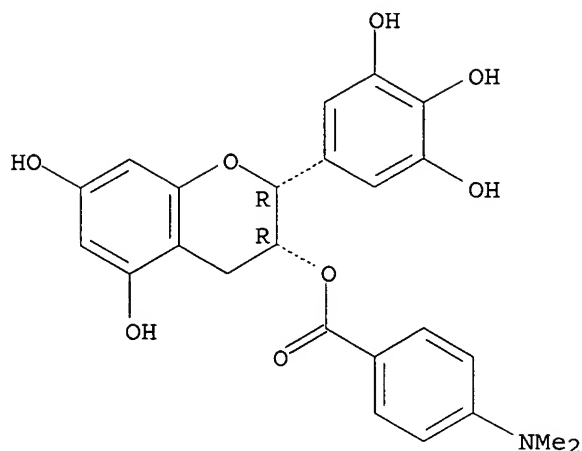
IT 224441-48-9, HZIV 92

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(HZIV 92; method and compns. for regulation of 5- α -reductase activity)

RN 224441-48-9 HCAPLUS

CN Benzoic acid, 4-(dimethylamino)-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 15 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:293978 HCAPLUS

DOCUMENT NUMBER: 136:337341

TITLE: Materials and methods to modulate ligand binding/enzymic activity of α/β proteins containing an allosteric regulatory site

INVENTOR(S): Stauton, Donald E.

PATENT ASSIGNEE(S): Icos Corporation, USA

SOURCE: PCT Int. Appl., 163 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002031511	A2	20020418	WO 2001-US32047	20011012
WO 2002031511	A3	20030313		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2425581	AA	20020418	CA 2001-2425581	20011012
AU 2002013196	A5	20020422	AU 2002-13196	20011012
US 2003088061	A1	20030508	US 2001-976935	20011012
EP 1325341	A2	20030709	EP 2001-981560	20011012
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2004511496	T2	20040415	JP 2002-534845	20011012
PRIORITY APPLN. INFO.:			US 2000-239750P	P 20001012
			WO 2001-US32047	W 20011012
AB	Methods of modulating binding between an α/β protein and a			

binding partner are provided, along with methods of identifying modulators and their use. The methods comprise contacting the α/β protein with an allosteric effector mol. which binds to an allosteric site of the α/β protein and alters the conformation of the α/β protein such that the binding of the α/β protein to a binding partner is modulated. Thus, a primary screen for inhibitors of the classical pathway complement protein C2 and alternative pathway complement protein factor B involving modifications of standard hemolytic CH50 and AH50 assays in a microtiter plate format was carried out. Lead compds. identified in this screen were submitted to a second screening using purified complement proteins to determine which stage of complement activation the compds. inhibited. Five diaryl sulfides were identified. Numerous other assays, e.g., to identify inhibitors of integrin $\alpha E\beta$ interaction with E cadherin, inhibitors of Rac1 GDP-GTP exchange, or antagonists of E. coli 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase, were conducted as well.

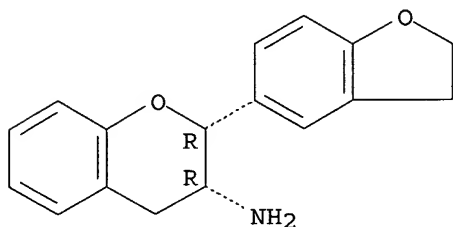
IT 415718-09-1

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(materials and methods to modulate ligand binding/enzymic activity of α/β proteins containing allosteric regulatory site)

RN 415718-09-1 HCAPLUS

CN 2H-1-Benzopyran-3-amine, 2-(2,3-dihydro-5-benzofuranyl)-3,4-dihydro-,
(2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L48 ANSWER 16 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:681413 HCAPLUS

DOCUMENT NUMBER: 135:242062

TITLE: Preparation of catechin derivatives with increased stability

INVENTOR(S): Miyase, Toshio; Sano, Mitsuaki

PATENT ASSIGNEE(S): Shizuoka Prefecture, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001253879	A2	20010918	JP 2000-112742	20000309
PRIORITY APPLN. INFO.:			JP 2000-112742	20000309
OTHER SOURCE(S): CASREACT 135:242062; MARPAT 135:242062				
AB The derivs. I (≥ 1 of R1-R7 = C1-10 alkyl; R8 = H, OH; the others = H, β -D-glucosyl), which have good absorbability and slow metabolic rate and are useful as antioxidants, apoptosis inducers, allergy				

inhibitors, etc. (no data), are prepared by treating catechins with C1-10 alkyl halides in the presence of Li_2CO_3 . A mixture of (-)-epigallocatechin-3-O-gallate (1.00 g), DMF, Li_2CO_3 , and MeI was stirred at room temperature for 24 h to give 365 mg (-)-epigallocatechin-3-O-(4-O-methyl)gallate.

IT 108907-44-4P 224434-07-5P 360059-38-7P

360059-39-8P

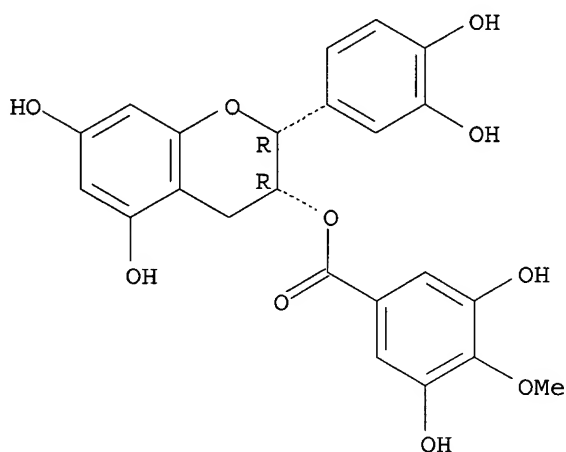
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of partial alkyl ethers of catechin gallates with increased stability using Li_2CO_3)

RN 108907-44-4 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

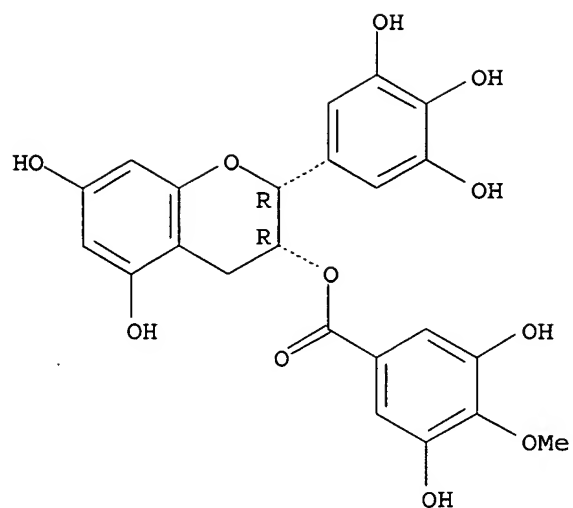
Absolute stereochemistry.



RN 224434-07-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

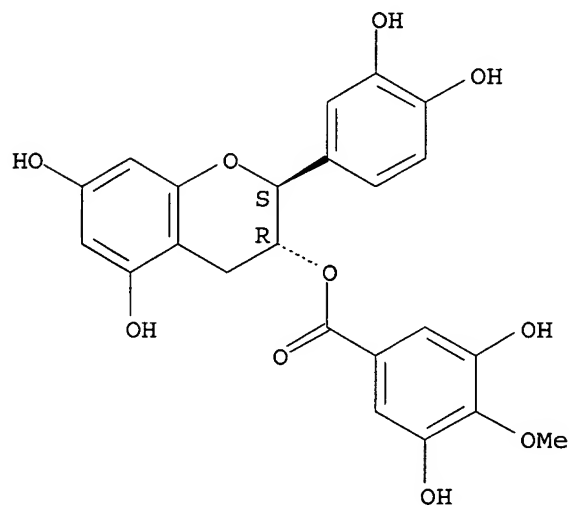
Absolute stereochemistry. Rotation (-).



RN 360059-38-7 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2S,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

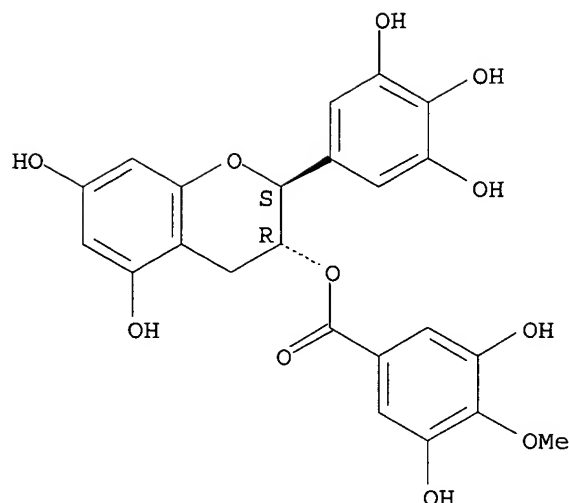
Absolute stereochemistry.



RN 360059-39-8 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2S,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 17 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:603497 HCAPLUS

DOCUMENT NUMBER: 135:175356

TITLE: Plant polyphenols as leukemia inhibitors

INVENTOR(S): Oba, Hideki; Nakamura, Osamu; Yasuda, Seiji; Moriwaki, Sawako; Tanaka, Takashi

PATENT ASSIGNEE(S): Ministry of Economy, Trade and Industry; National Industrial Research Institute, Japan; National Institute of Advanced Industrial Science and Technology

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE: **Patent**

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001226276	A2	20010821	JP 2000-38873	20000216
JP 3525182	B2	20040510		

PRIORITY APPLN. INFO.: JP 2000-38873 20000216

AB Plant polyphenols from green tea, cinnamon bark, and Paeonia lactiflora roots are claimed as leukemia inhibitors by inducing apoptosis of the leukemia cells.

IT **355120-39-7**

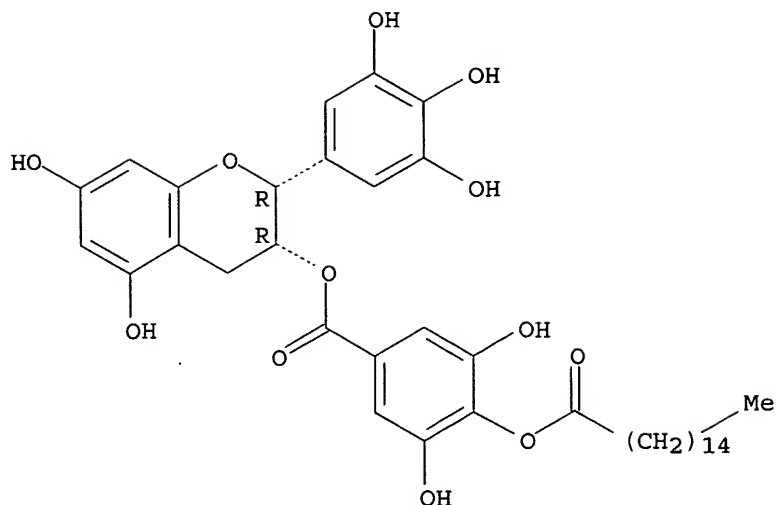
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(plant polyphenols as leukemia inhibitors)

RN 355120-39-7 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-[(1-oxohexadecyl)oxy]-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 18 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STM

ACCESSION NUMBER: 2000:388871 HCAPLUS

DOCUMENT NUMBER: 133:22185

TITLE: Anti-allergy and anti-inflammatory catechins from tea extracts

INVENTOR(S): Tsuji, Akimitsu; Yamamoto, Mari; Kawahara, Kouji; Sano, Mitsuaki; Miyase, Toshio

PATENT ASSIGNEE(S): Norinsuisansho Yasai Chagyo Shikenjocho, Japan; Seibutsu Kei Tokutei Sangyo Gijutsu Kenkyu Suishin Kiko; Shizuoka Prefecture; National Institute of Agro-Environmental Sciences

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000159670	A2	20000613	JP 1998-346646	19981120
JP 3637355	B2	20050413		
EP 1157693	A1	20011128	EP 2000-110160	20000512

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

PRIORITY APPLN. INFO.: JP 1998-346646 A 19981120

AB This invention relates to antiallergy and antiinflammatory agents comprising 3-O-methylgalloylepigallocatechin (I) and/or 4-O-methylgalloylepigallocatechin (II). The agents can be administered topically or orally. I and II were isolated from polyphenol fractions of MeOH exts. of tea leaves. Candies, chewing gums, and bath preps. containing the invention compds. were formulated.

IT 83104-87-4 224434-07-5

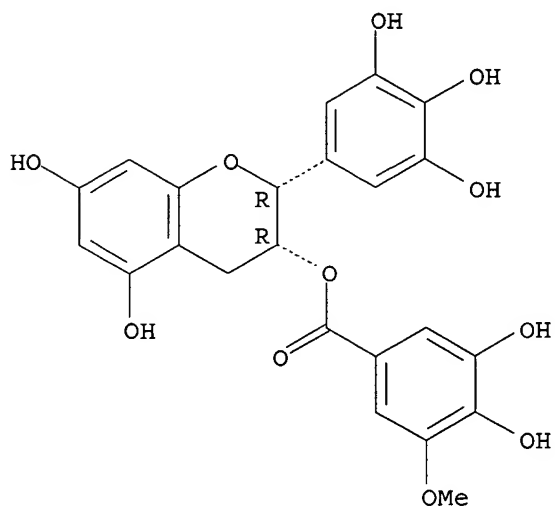
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BUU (Biological use, unclassified); FFD (Food or feed use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)

(anti-allergy and anti-inflammatory catechins from tea exts.)

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

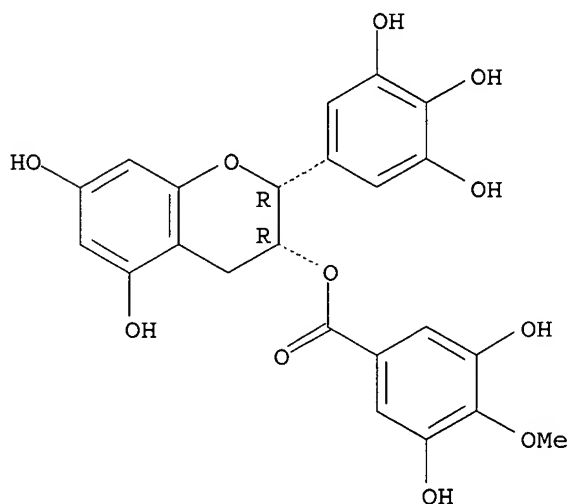
Absolute stereochemistry. Rotation (-).



RN 224434-07-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L48 ANSWER 19 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:311102 HCAPLUS

DOCUMENT NUMBER: 130:332910

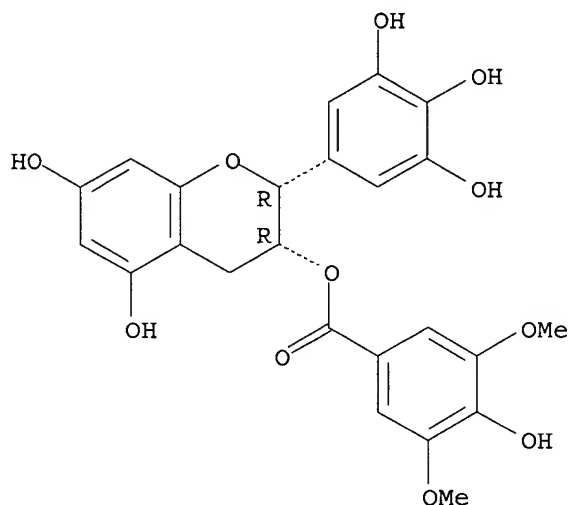
TITLE: Methods and compositions for regulation of 5-alpha

reductase activity
 INVENTOR(S): Liao, Shutsung; Hiipakka, Richard A.
 PATENT ASSIGNEE(S): Arch Development Corporation, USA
 SOURCE: PCT Int. Appl., 48 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 8
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9922728	A1	19990514	WO 1998-US23041	19981030
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
AU 9912898	A1	19990524	AU 1999-12898	19981030
EP 1027045	A1	20000816	EP 1998-956358	19981030
R:	AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, SE, PT, IE			
JP 2003524577	T2	20030819	JP 2000-518662	19981030
US 6576660	B1	20030610	US 2000-530443	20000428
US 2003105030	A1	20030605	US 2002-132050	20020424
US 6696484	B2	20040224		
US 2003153541	A1	20030814	US 2002-174934	20020619
US 2003144346	A1	20030731	US 2002-294331	20021114
PRIORITY APPLN. INFO.:			US 1997-63770P	P 19971031
			WO 1998-US23041	W 19981030
			US 1999-131728P	P 19990430
			US 2000-530443	A2 20000428
			US 2000-560236	A2 20000428
			US 2001-267493P	P 20010208
			US 2001-288643P	P 20010503
			US 2001-348020P	P 20011108
			US 2002-72128	A2 20020208
			US 2002-137695	A2 20020502
OTHER SOURCE(S):	MARPAT 130:332910			
AB	Compds. that inhibit 5 α -reductase are provided. The compds. are used to treat prostate cancer, breast cancer, obesity, skin disorders and baldness.			
IT	173484-92-9, HZIV 75 183209-70-3, HZIV 145 224433-76-5, HZIV 120 224433-78-7, HZIV 166 224441-44-5, HZIV 160 224441-46-7, HZIV 134 224441-48-9, HZIV 92 224441-50-3, HZIV 142 224441-52-5, HZIV 68 224441-56-9, HZIV 169 224441-58-1, HZIV 74 224441-60-5, HZIV 144 224441-61-6, HZIV 168 224441-64-9, HZIV 107 224441-66-1, HZIV 148 224441-68-3, HZIV 109 224441-70-7, HZIV 165			
RL:	BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)			
	(steroid 5- α reductase inhibitors, and therapeutic use)			
RN	173484-92-9 HCAPLUS			
CN	Benzoic acid, 4-hydroxy-3,5-dimethoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-			

2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

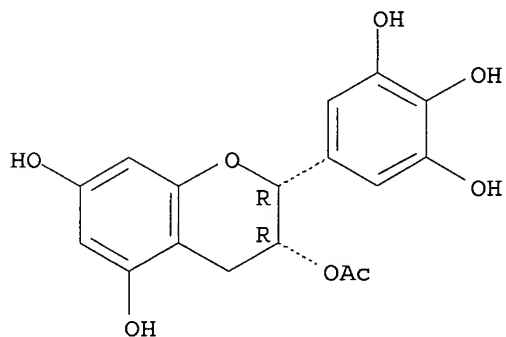
Absolute stereochemistry.



RN 183209-70-3 HCAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, 3-acetate, (2R,3R)- (9CI) (CA INDEX NAME)

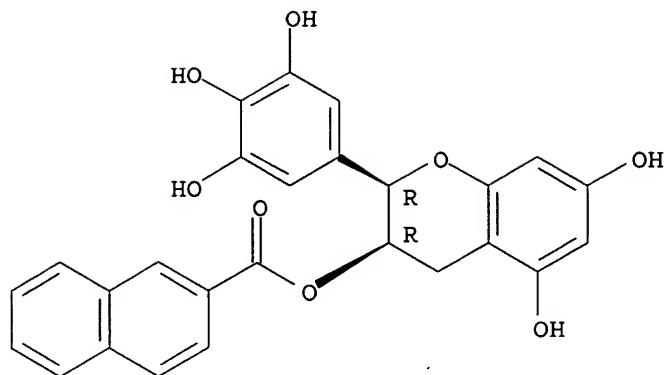
Absolute stereochemistry.



RN 224433-76-5 HCAPLUS

CN 2-Naphthalenecarboxylic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

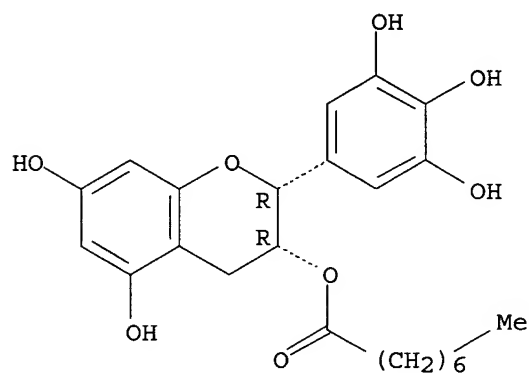
Absolute stereochemistry.



RN 224433-78-7 HCAPLUS

CN Octanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

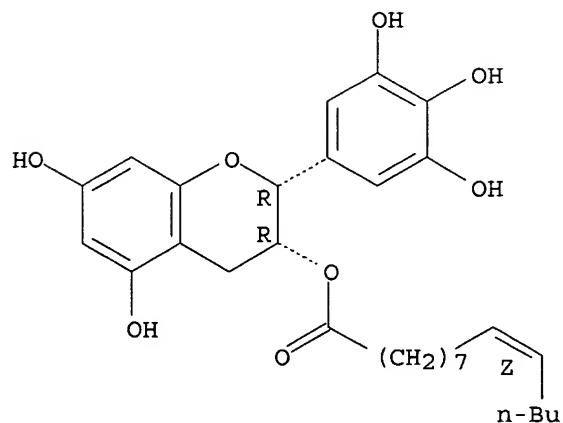
Absolute stereochemistry. Rotation (-).



RN 224441-44-5 HCAPLUS

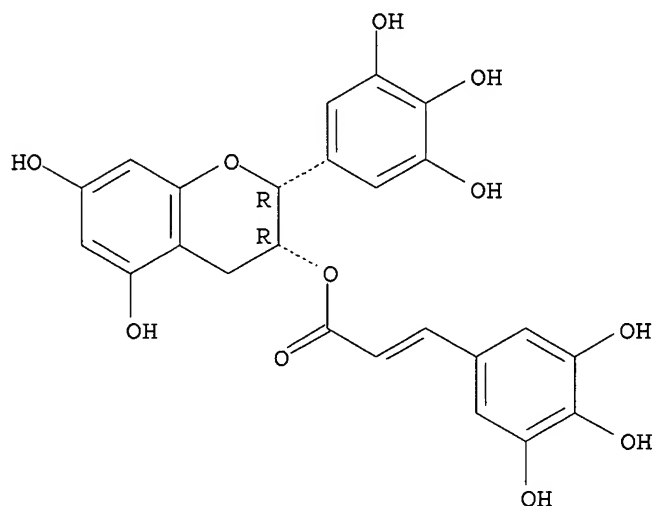
CN 9-Tetradecenoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, (9Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



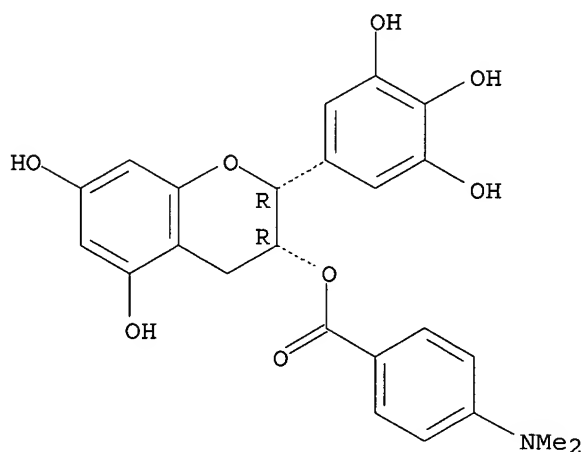
RN 224441-46-7 HCAPLUS
CN 2-Propenoic acid, 3-(3,4,5-trihydroxyphenyl)-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.
Currently available stereo shown.



RN 224441-48-9 HCAPLUS
CN Benzoic acid, 4-(dimethylamino)-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

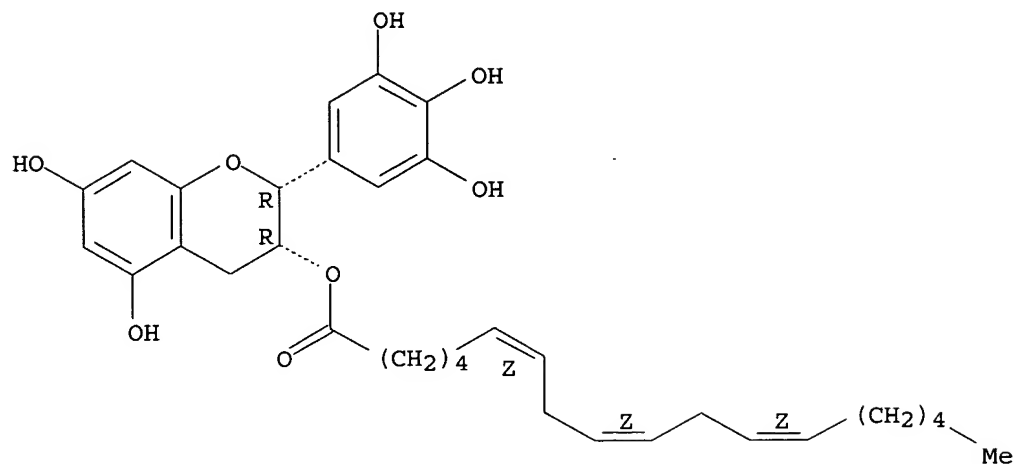
Absolute stereochemistry.



RN 224441-50-3 HCAPLUS
CN 6,9,12-Octadecatrienoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, (6Z,9Z,12Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

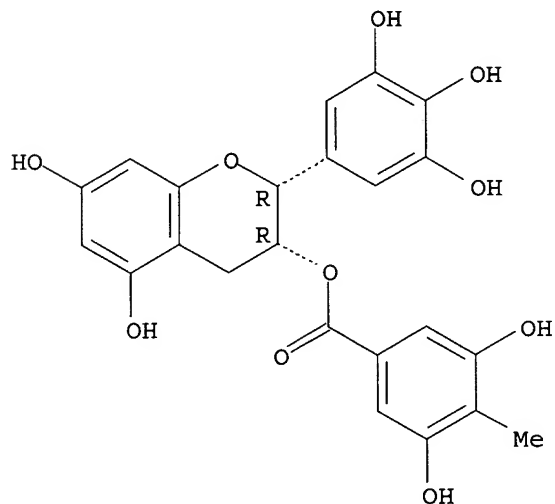
Double bond geometry as shown.



RN 224441-52-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methyl-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

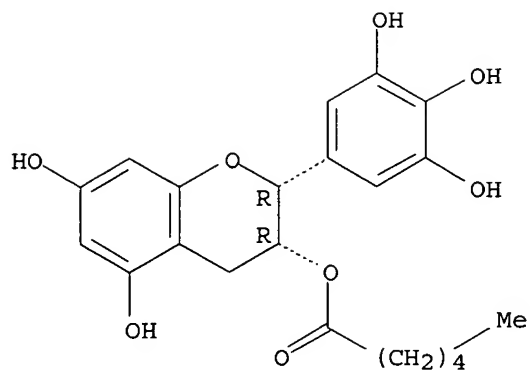
Absolute stereochemistry.



RN 224441-56-9 HCAPLUS

CN Hexanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

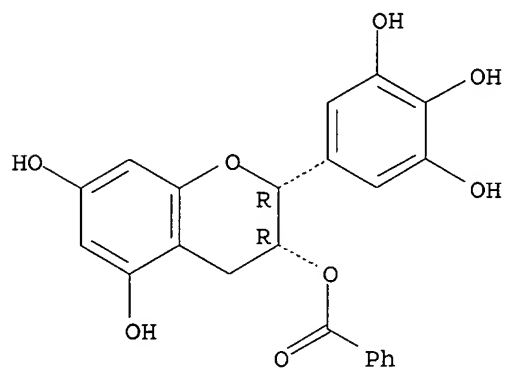
Absolute stereochemistry. Rotation (-).



RN 224441-58-1 HCAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, 3-benzoate, (2R,3R)- (9CI) (CA INDEX NAME)

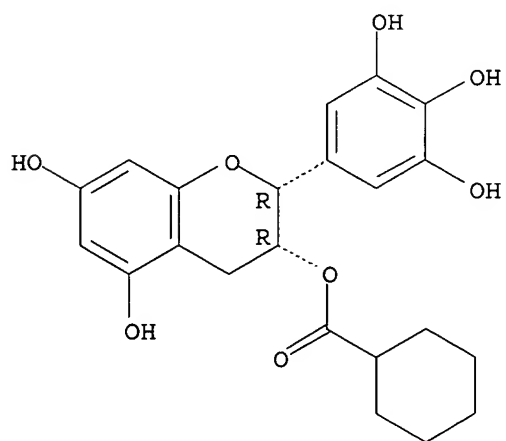
Absolute stereochemistry.



RN 224441-60-5 HCAPLUS

CN Cyclohexanecarboxylic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

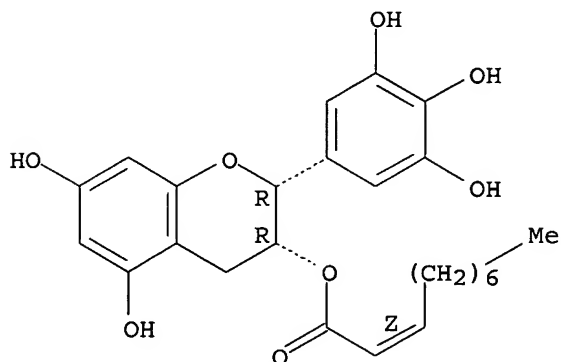
Absolute stereochemistry.



RN 224441-61-6 HCAPLUS

CN 2-Decenoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, (2Z)- (9CI) (CA INDEX NAME)

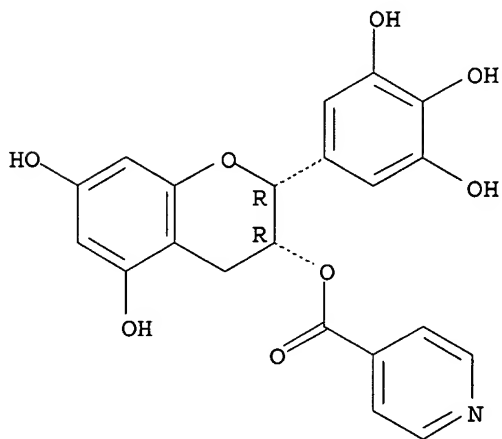
Absolute stereochemistry.
Double bond geometry as shown.



RN 224441-64-9 HCAPLUS

CN 4-Pyridinecarboxylic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

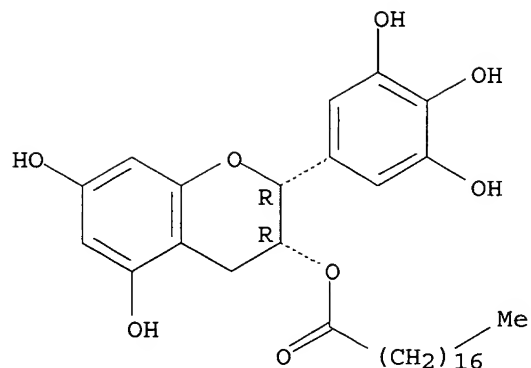
Absolute stereochemistry.



RN 224441-66-1 HCAPLUS

CN Octadecanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

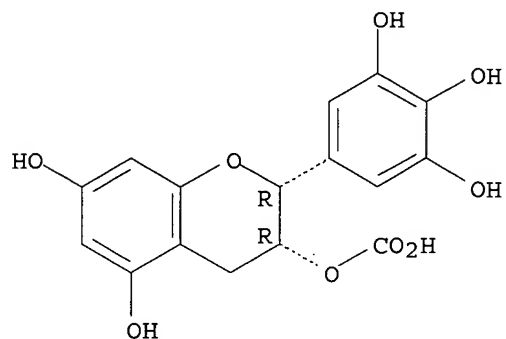
Absolute stereochemistry. Rotation (-).



RN 224441-68-3 HCAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, 3-(hydrogen carbonate), (2R,3R)- (9CI) (CA INDEX NAME)

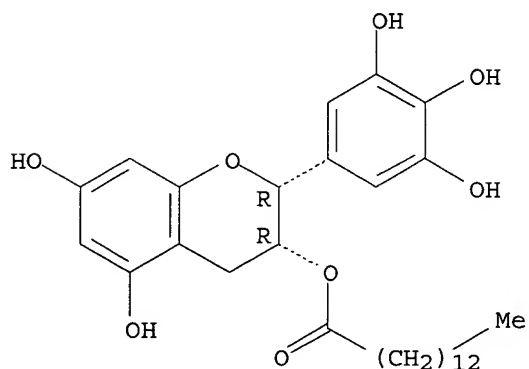
Absolute stereochemistry.



RN 224441-70-7 HCAPLUS

CN Tetradecanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 20 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:627426 HCAPLUS

DOCUMENT NUMBER: 129:267845

TITLE: Silver halide photographic material with improved storage stability

INVENTOR(S): Ono, Koji

PATENT ASSIGNEE(S): Konica Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 30 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10254087	A2	19980925	JP 1997-60848	19970314
PRIORITY APPLN. INFO.:			JP 1997-60848	19970314
OTHER SOURCE(S): MARPAT 129:267845				

AB The title material, possessing ≥ 1 Ag halide emulsion layer on a support, employs Ag halide grains having the spectral maximum sensitivity in the range of 700-1500 nm and contains ≥ 1 compound I [R1, R2 = OH, SH, (substituted) amino, acylamino alkylsulfonylamino, arylsulfonylamino, alkoxycarbonyl, alkylthio; Z = atomic group forming (substituted) 5- or 6-membered ring] and ≥ 1 compds. selected from heterocycles II (Z1 = atoms required to form a heterocycle containing ≥ 1 N atom; X = N or methine group) and III (R3 = H or OH; R4 = H, IV; R5 = H, OH) in the emulsion layer and/or its adjacent hydrophilic colloid layer. The material shows high sensitivity toward laser beams and excellent storage stability.

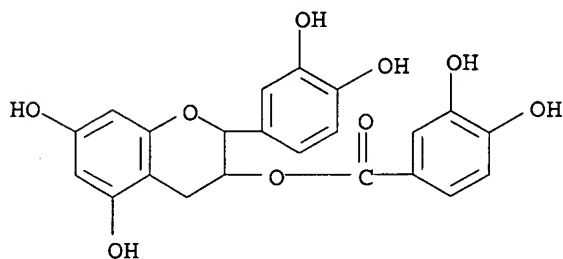
IT 213598-37-9 213598-38-0

RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)

(photog. emulsion containing additives for improving laser selectivity and storage stability)

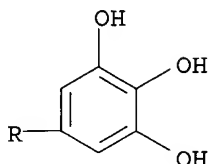
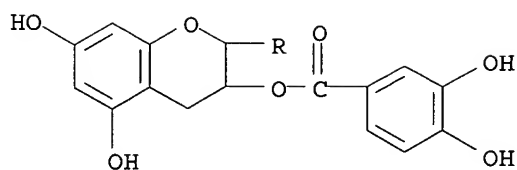
RN 213598-37-9 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)



RN 213598-38-0 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-, 3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)



L48 ANSWER 21 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1998:627425 HCAPLUS
 DOCUMENT NUMBER: 129:308482
 TITLE: Silver halide photographic photosensitive material
 with improved storage stability
 INVENTOR(S): Ono, Koji
 PATENT ASSIGNEE(S): Konica Co., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 27 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: **Patent**
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10254086	A2	19980925	JP 1997-59358	19970313
PRIORITY APPLN. INFO.:			JP 1997-59358	19970313

OTHER SOURCE(S): MARPAT 129:308482

AB The title material, possessing ≥ 1 Ag halide emulsion layer on a support, employs Ag halide grains having the spectral maximum sensitivity in the range of 700-1500 nm and contains ≥ 1 pyrazolidone-type compound I (R = aryl; R1-4 = H, alkyl, aralkyl, aryl) and ≥ 1 compds. selected from heterocycles II (Z1 = atoms required to form a heterocycle containing ≥ 1 N atom; X = N or methine group) and III (R3 = H or OH; R4 = H, IV; R5 = H, OH) in the emulsion layer and/or its adjacent hydrophilic colloid layer. The material shows high sensitivity toward laser beams and excellent storage stability.

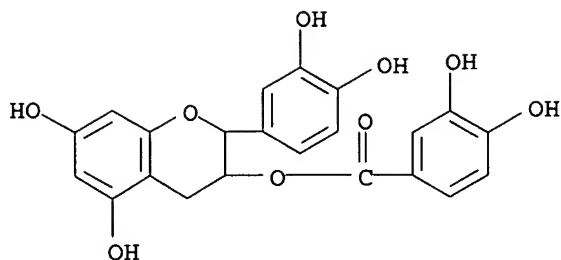
IT 213598-37-9 213598-38-0

RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)

(in silver halide emulsion containing pyrazolidones with high laser sensitivity and storage stability)

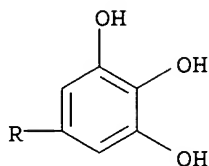
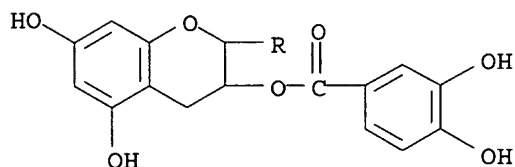
RN 213598-37-9 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)



RN 213598-38-0 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-, 3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)



L48 ANSWER 22 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:20761 HCAPLUS

DOCUMENT NUMBER: 126:59804

TITLE: Preparation of (2S)-trans-3-(acyloxy)flavans as intermediates for optically active (2S)-trans-3-hydroxyflavan derivatives

INVENTOR(S): Izumi, Taeko

PATENT ASSIGNEE(S): Kawaken Fine Chemicals Co, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08259555	A2	19961008	JP 1995-61028	19950320

PRIORITY APPLN. INFO.: JP 1995-61028 19950320

OTHER SOURCE(S): MARPAT 126:59804

AB The title compds. [I; II; X, Y = H; or XY = O; Z = C1-6 alkyl, C1-6 alkenyl, Ph, halo, etc.; R1-R8 = H, halo, OH, alkyl, alkoxy, etc.] are prepared. Thus, (±)-trans-3-hydroxyflavan in iso-Pr ether containing lipase PC and mol. sieves 4A was reacted with vinyl acetate to give (-)-(2S,3R)-trans-3-acetoxyflavan (III) and (-)-(2R,3S)-trans-3-

hydroxyflavan. III was refluxed with methanol containing 10% HCl to give (+)-(2S,3R)-trans-3-hydroxyflavan.

IT 184713-80-2P, (-)-(2S,3R)-trans-3-Acetoxyflavan
184713-83-5P

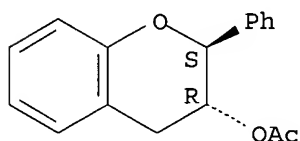
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2S-trans(acyloxy)flavans as intermediates for optically active 2S-trans-hydroxyflavan derivs.)

RN 184713-80-2 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 3,4-dihydro-2-phenyl-, acetate, (2S-trans)- (9CI)
(CA INDEX NAME)

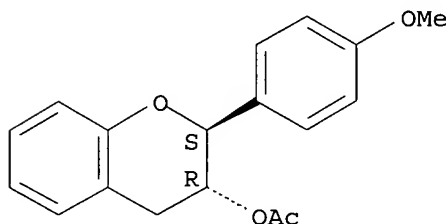
Absolute stereochemistry. Rotation (-).



RN 184713-83-5 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 3,4-dihydro-2-(4-methoxyphenyl)-, acetate, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 132199-49-6P 184713-82-4P 184713-86-8P

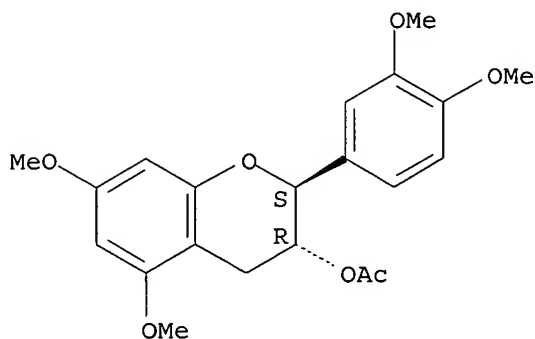
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of 2S-trans(acyloxy)flavans as intermediates for optically active 2S-trans-hydroxyflavan derivs.)

RN 132199-49-6 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-5,7-dimethoxy-, acetate, (2S,3R)- (9CI) (CA INDEX NAME)

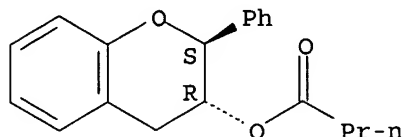
Absolute stereochemistry. Rotation (-).



RN 184713-82-4 HCAPLUS

CN Butanoic acid, 3,4-dihydro-2-phenyl-2H-1-benzopyran-3-yl ester,
(2S-trans)- (9CI) (CA INDEX NAME)

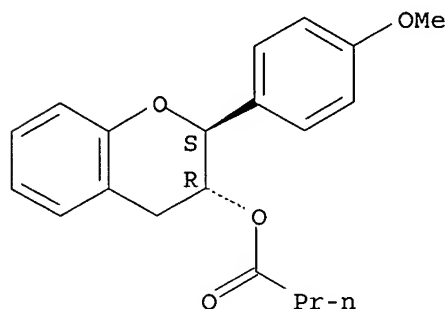
Absolute stereochemistry. Rotation (-).



RN 184713-86-8 HCAPLUS

CN Butanoic acid, 3,4-dihydro-2-(4-methoxyphenyl)-2H-1-benzopyran-3-yl ester,
(2S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L48 ANSWER 23 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:219132 HCAPLUS

DOCUMENT NUMBER: 122:9870

TITLE: Preparation of 3-acylated catechins as antioxidative agents

INVENTOR(S): Sakai, Miwa; Suzuki, Masayuki; Nanjo, Fumio; Hara, Yukihiro

PATENT ASSIGNEE(S): Mitsui Norin Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 7 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 618203	A1	19941005	EP 1994-104887	19940328
R: AT, BE, CH, DE, DK, ES, FR, GB, IE, IT, LI, LU, NL, SE				
JP 06279430	A2	19941004	JP 1993-91934	19930329
JP 3165279	B2	20010514		

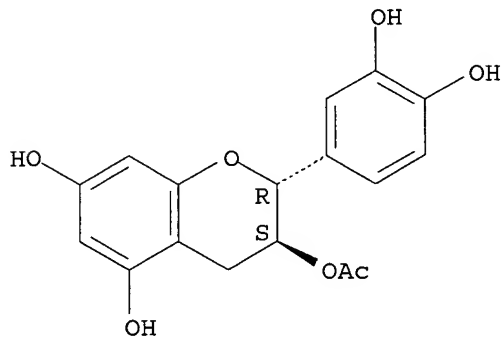
PRIORITY APPLN. INFO.: JP 1993-91934 A 19930329

OTHER SOURCE(S): MARPAT 122:9870

AB Title compds. I (X = C1-10 alkyl, R = H, HO) are prepared by an efficient method with superior oil solubility, by using transesterification by carboxyesterase. Carboxyesterase, (-)-catechin and EtOAc were reacted for

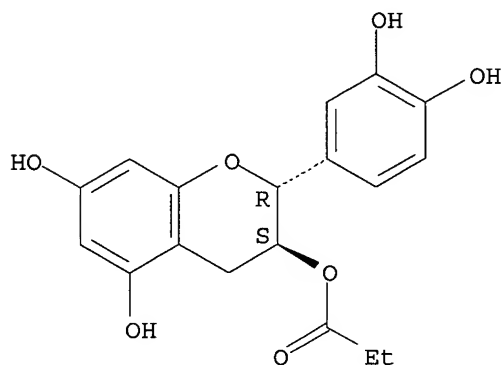
24 h at 33° to give after workup, (-)-I (X = Me, R = H).
 IT 116935-88-7P, (-)-3-O-Acetylcathechin 159333-36-5P
 159333-37-6P 159333-38-7P
 RL: IMF (Industrial manufacture); MOA (Modifier or additive use); SPN
 (Synthetic preparation); PREP (Preparation); USES (Uses)
 (preparation of 3-acylated catechins as antioxidative agents)
 RN 116935-88-7 HCAPLUS
 CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-,
 3-acetate, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



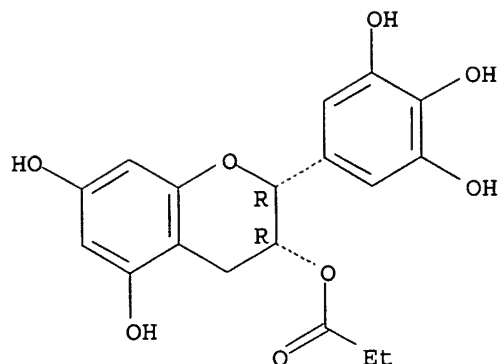
RN 159333-36-5 HCAPLUS
 CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-,
 3-propanoate, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



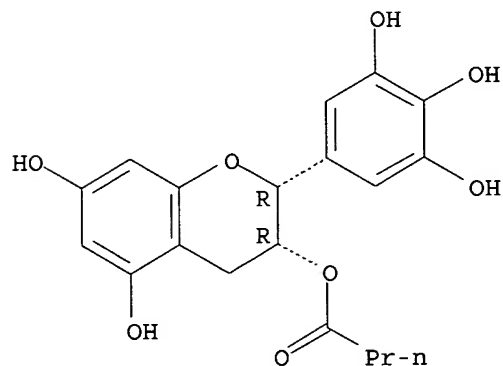
RN 159333-37-6 HCAPLUS
 CN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-,
 3-propanoate, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159333-38-7 HCAPLUS
 CN Butanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L48 ANSWER 24 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1984:138846 HCAPLUS
 DOCUMENT NUMBER: 100:138846
 TITLE: (+)-Cyanidan-3-ol derivatives pharmaceutical preparations
 INVENTOR(S): Albert, Alban Imre; Ballenegger, Marc Ernest; Overeem, Jan Cornelis; Tyson, Robert Graham
 PATENT ASSIGNEE(S): Zyma S. A., Switz.
 SOURCE: Eur. Pat. Appl., 48 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
EP 96008	A2	19831207	EP 1983-810223	19830526
EP 96008	A3	19840111		
EP 96008	B1	19890329		
R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
GB 2122987	A1	19840125	GB 1983-12766	19830510

GB 2122987	B2	19850925		
AT 41774	E	19890415	AT 1983-810223	19830526
FI 8301927	A	19831202	FI 1983-1927	19830530
ZA 8303905	A	19840125	ZA 1983-3905	19830530
ES 522815	A1	19850201	ES 1983-522815	19830530
CA 1252108	A1	19890404	CA 1983-429164	19830530
DK 8302453	A	19831202	DK 1983-2453	19830531
NO 8301951	A	19831202	NO 1983-1951	19830531
NO 158805	B	19880725		
NO 158805	C	19881101		
AU 8315256	A1	19831208	AU 1983-15256	19830531
AU 569033	B2	19880121		
JP 58219184	A2	19831220	JP 1983-96841	19830531
HU 31226	O	19840428	HU 1983-1942	19830531
HU 193537	B	19871028		
DD 210042	A5	19840530	DD 1983-251544	19830531
US 4510159	A	19850409	US 1983-499644	19830531
IL 68833	A1	19871030	IL 1983-68833	19830531
PRIORITY APPLN. INFO.:			GB 1982-15868	A 19820601
			EP 1983-810223	A 19830526

OTHER SOURCE(S): CASREACT 100:138846

AB Cyanidanols I [R, R1 = H, (un)substituted hydrocarbon, acyl; R2, R3 = H, (un)substituted hydrocarbon; R2R3 = alkylene] were prepared Thus, (+)-cyanidan-3-ol was treated with Ph₂CCl₂ to give I (R = R1 = H, R2 = R3 = Ph), which at 50 mg/kg gave 31.6% inhibition of D-galactosamine edema.

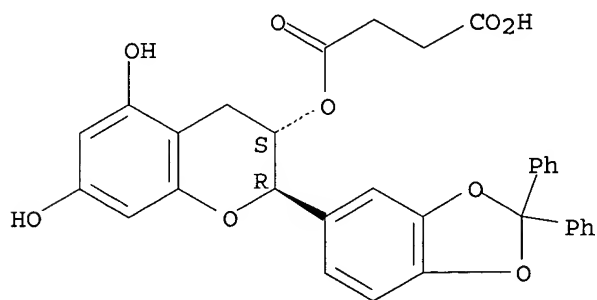
IT 89329-13-5P 89329-15-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 89329-13-5 HCAPLUS

CN Butanedioic acid, mono[2-(2,2-diphenyl-1,3-benzodioxol-5-yl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl] ester, (2R-trans)- (9CI) (CA INDEX NAME)

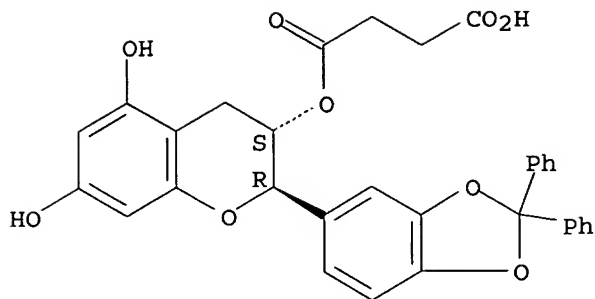
Absolute stereochemistry.



RN 89329-15-7 HCAPLUS

CN Butanedioic acid, mono[2-(2,2-diphenyl-1,3-benzodioxol-5-yl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl] ester, monosodium salt, (2R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Na

L48 ANSWER 25 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1983:53519 HCAPLUS
 DOCUMENT NUMBER: 98:53519
 TITLE: Catechin derivatives
 PATENT ASSIGNEE(S): Kanebo, Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57118580	A2	19820723	JP 1981-5571	19810116
PRIORITY APPLN. INFO.:			JP 1981-5571	19810116
OTHER SOURCE(S): CASREACT 98:53519				

AB Twenty-six catechin derivs. (+)-I (R, R1, R2 = H, alkyl, acyl) were prepared by selective acylation of the 5- and 7-positions in catechins optionally followed by proper chemical treatments. Anticarcinogenic test data of I were shown against Ehrlich ascite tumor in mice. Thus, 10.2 g BzCl was added to an aqueous mixture of 11.61 g (+)-catechin and 24.7 mg H3BO3 (adjusted to pH 8.6 with 2N aqueous NaOH) with ice cooling by keeping pH 8.5-9.0 to give, after 1 h, 38% (+)-I (R = Bz, R1 = R2 = H).

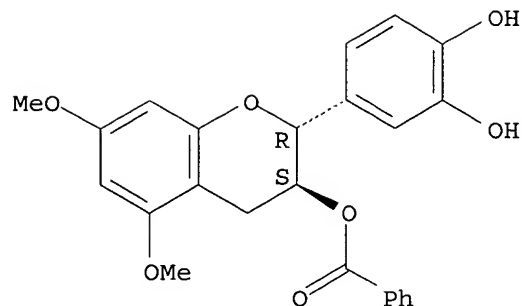
IT 84188-73-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation and antineoplastic activity of)

RN 84188-73-8 HCAPLUS

CN 1,2-Benzenediol, 4-[3-(benzoyloxy)-3,4-dihydro-5,7-dimethoxy-2H-1-benzopyran-2-yl]-, (2R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 26 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1982:40929 HCAPLUS

DOCUMENT NUMBER: 96:40929

TITLE: Use of O-substituted (+)-3-cyanidanol derivatives as compounds with immunomodulative properties

INVENTOR(S): Courbat, Pierre; Weith, Andre; Albert, Alban

PATENT ASSIGNEE(S): Zyma S. A., Switz.

SOURCE: Eur. Pat. Appl., 34 pp.

CODEN: EPXXDW

DOCUMENT TYPE: **Patent**

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 37800	A2	19811014	EP 1981-810130	19810331
EP 37800	A3	19811021		
EP 37800	B1	19870812		
R: CH, DE, FR, GB, LU, SE				
BE 888244	A1	19811002	BE 1981-204352	19810402
AU 8169032	A1	19811008	AU 1981-69032	19810402
AU 548310	B2	19851205		
NL 8101648	A	19811102	NL 1981-1648	19810402
JP 56154415	A2	19811130	JP 1981-49494	19810403
US 4634718	A	19870106	US 1986-834507	19860228

PRIORITY APPLN. INFO.:

CH 1980-2679	A	19800403
US 1981-247961	A1	19810326
US 1983-531809	A1	19830825
US 1985-713561	A1	19850318

AB (+)-Cyanidanol derivs. (I, R = C_{≥2} acyl, alkyl, organic sulfonic acid or inorg. acid containing more than one O) have immunomodulating properties and are used for the treatment of mammalian diseases such as leukemia. Tablets were prepared each containing 250 mg 3-O-palmitoyl-(+)-3-cyanidanol

(II) [71634-82-7]. I antitumor properties in rats were described.

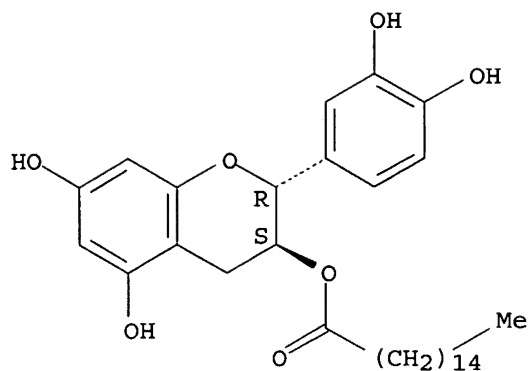
IT 71634-82-7 71634-84-9 80500-87-4

RL: BIOL (Biological study)
(antitumor pharmaceuticals containing)

RN 71634-82-7 HCAPLUS

CN Hexadecanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

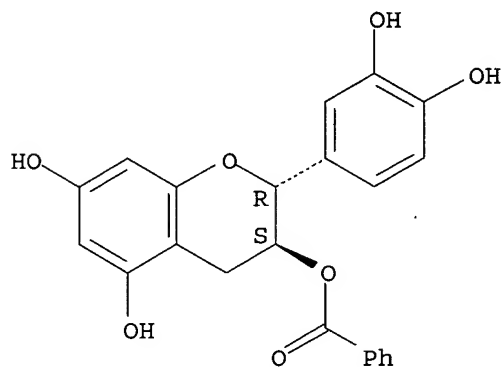
Absolute stereochemistry.



RN 71634-84-9 HCAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-,
3-benzoate, (2R-trans)- (9CI) (CA INDEX NAME)

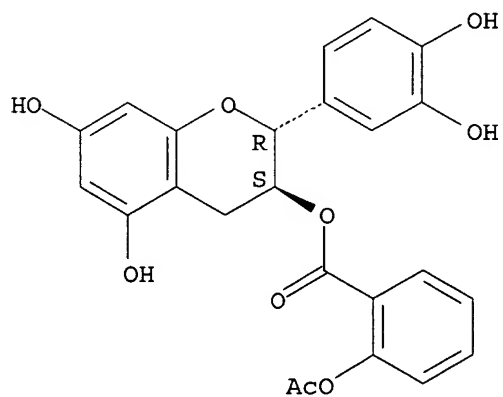
Absolute stereochemistry.



RN 80500-87-4 HCAPLUS

CN Benzoic acid, 2-(acetyloxy)-, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-
dihydroxy-2H-1-benzopyran-3-yl ester, (2R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 27 OF 27 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1979:575201 HCAPLUS
 DOCUMENT NUMBER: 91:175201
 TITLE: O-Substituted (+)-cyanidan-3-ols
 PATENT ASSIGNEE(S): Zyma S. A., Switz.
 SOURCE: Jpn. Kokai Tokkyo Koho, 38 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54081274	A2	19790628	JP 1978-145940	19781125
EP 39844	A2	19811118	EP 1981-103265	19781112
EP 39844	A3	19811122		
R: BE, CH, DE, FR, GB, LU, NL, SE				
US 4255336	A	19810310	US 1978-962743	19781121
EP 3274	A1	19790808	EP 1978-810024	19781122
EP 3274	B1	19840229		
R: BE, CH, DE, FR, GB, LU, NL, SE				
CS 228112	P	19840514	CS 1978-7628	19781122
FI 7803593	A	19790526	FI 1978-3593	19781123
ES 475338	A1	19800301	ES 1978-475338	19781123
AT 7808356	A	19810415	AT 1978-8356	19781123
AT 364835	B	19811125		
AU 526985	B2	19830210	AU 1978-41877	19781123
AU 7841877	A1	19790531		
CA 1171423	A1	19840724	CA 1978-316769	19781123
IL 56030	A1	19850830	IL 1978-56030	19781123
DK 7805257	A	19790526	DK 1978-5257	19781124
NO 7803968	A	19790528	NO 1978-3968	19781124
NO 152651	B	19850722		
NO 152651	C	19851030		
ZA 7806638	A	19791128	ZA 1978-6638	19781124
PL 117814	B1	19810831	PL 1978-216715	19781124
PL 120640	B1	19820331	PL 1978-211196	19781124
HU 24302	O	19830128	HU 1978-ZI189	19781124
HU 183051	B	19840428		
HU 30743	O	19840328	HU 1982-3619	19781124
DD 141833	C	19800521	DD 1978-209343	19781127
DD 148055	C	19810506	DD 1978-217791	19781127
ES 480605	A1	19800401	ES 1979-480605	19790516
AT 8004640	A	19810415	AT 1980-4640	19800916
AT 364836	B	19811125		
CS 228139	P	19840514	CS 1980-6984	19801015
NO 8300800	A	19790528	NO 1983-800	19830308
US 4617296	A	19861014	US 1984-626823	19840702
PRIORITY APPLN. INFO.:			CH 1977-14479	A 19771125
			CH 1978-2937	A 19780317
			US 1978-962743	A3 19781121
			CS 1978-7628	A3 19781122
			EP 1978-810024	19781122
			AT 1978-8356	A 19781123
			US 1980-182169	A3 19800828
			US 1982-422110	A1 19820923
AB			Cyanidanols I [R = (substituted) hydrocarbon group, acyl, sulfonyl, except glycoside group; R1 = H] (II) and their salts were prepared from I (R as	

above, R1 = protective group). II and their salts are antihepatitis agents (0.1-0.5 g/kg). Thus, hydrogenating (+)-I (R = Me, R1 = PhCH₂) with Pd black in AcOEt gave quant. (+)-II (R = Me).

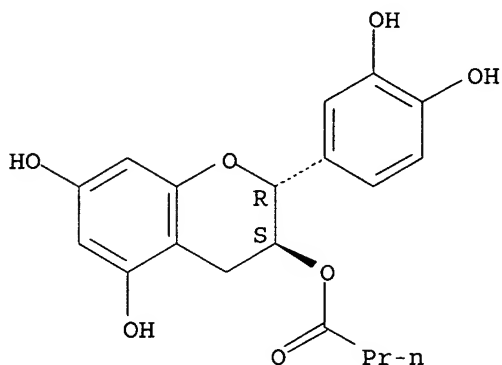
IT 71634-78-1P 71634-79-2P 71634-80-5P
71634-81-6P 71634-82-7P 71634-83-8P
71634-84-9P 71634-85-0P 71634-86-1P
71634-88-3P 71634-89-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antihepatitis activity of)

RN 71634-78-1 HCAPLUS

CN Butanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

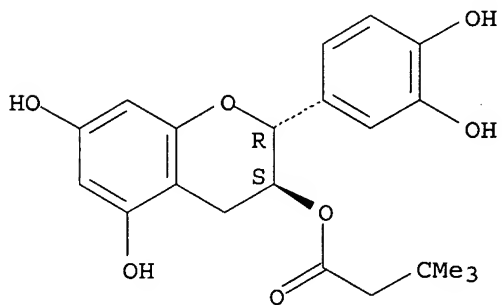
Absolute stereochemistry. Rotation (+).



RN 71634-79-2 HCAPLUS

CN Butanoic acid, 3,3-dimethyl-, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester, (2R-trans)- (9CI) (CA INDEX NAME)

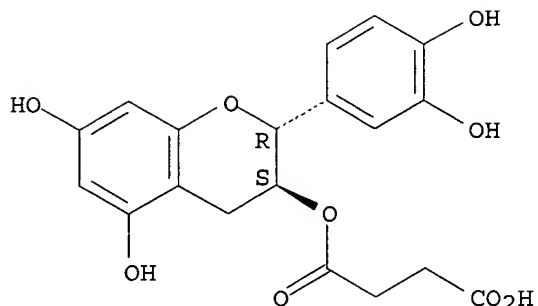
Absolute stereochemistry.



RN 71634-80-5 HCAPLUS

CN Butanedioic acid, mono[2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl] ester, (2R-trans)- (9CI) (CA INDEX NAME)

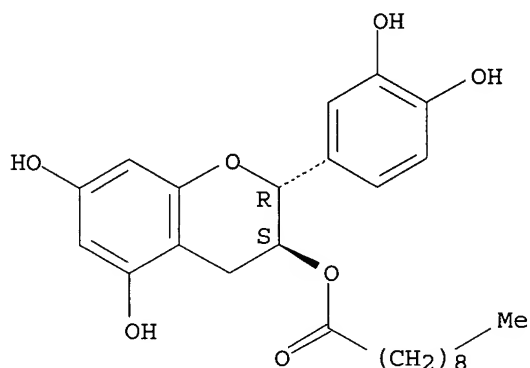
Absolute stereochemistry.



RN 71634-81-6 HCAPLUS

CN Decanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

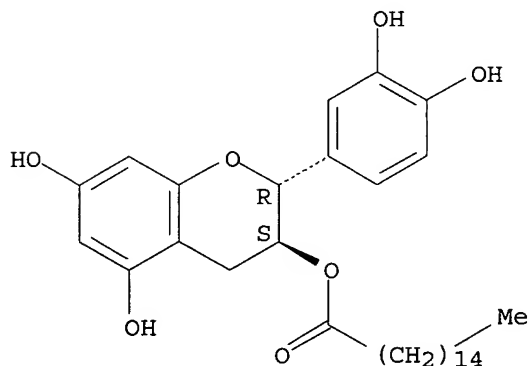
Absolute stereochemistry. Rotation (+).



RN 71634-82-7 HCAPLUS

CN Hexadecanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

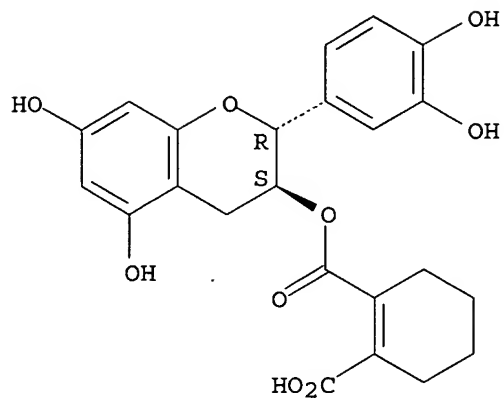
Absolute stereochemistry.



RN 71634-83-8 HCAPLUS

CN 1-Cyclohexene-1,2-dicarboxylic acid, mono[2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl] ester, (2R-trans)- (9CI) (CA INDEX NAME)

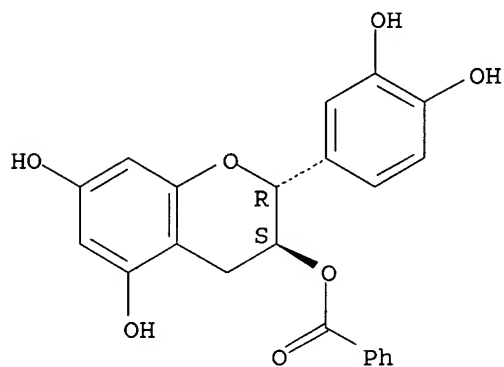
Absolute stereochemistry.



RN 71634-84-9 HCAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-,
3-benzoate, (2R-trans)- (9CI) (CA INDEX NAME)

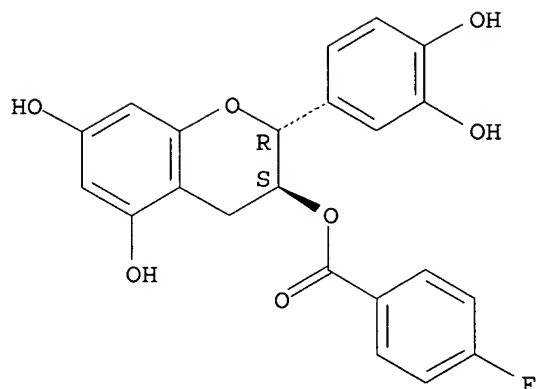
Absolute stereochemistry.



RN 71634-85-0 HCAPLUS

CN Benzoic acid, 4-fluoro-, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-
2H-1-benzopyran-3-yl ester, (2R-trans)- (9CI) (CA INDEX NAME)

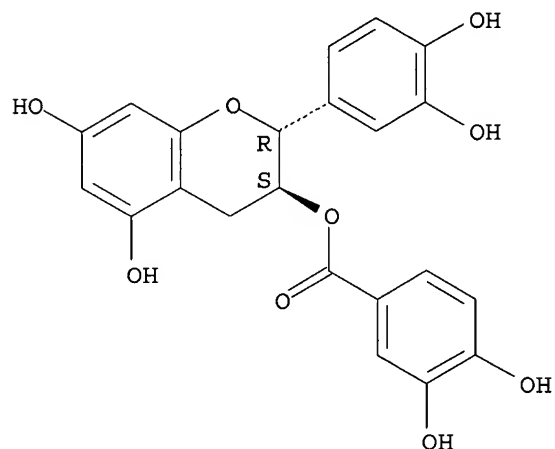
Absolute stereochemistry.



RN 71634-86-1 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester, (2R-trans)- (9CI) (CA INDEX NAME)

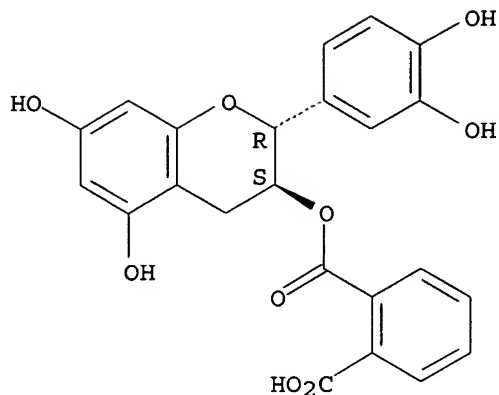
Absolute stereochemistry.



RN 71634-88-3 HCAPLUS

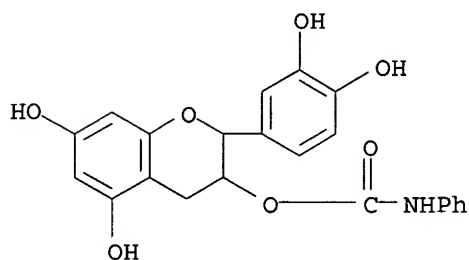
CN 1,2-Benzenedicarboxylic acid, mono[2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl] ester, (2R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 71634-89-4 HCAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-,
3-(phenylcarbamate), (2R-trans)- (9CI) (CA INDEX NAME)



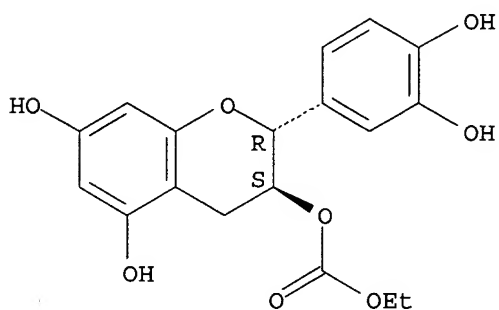
IT 71627-87-7P 71627-91-3P 71627-94-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 71627-87-7 HCAPLUS

CN Carbonic acid, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-
benzopyran-3-yl ethyl ester, (2R-trans)- (9CI) (CA INDEX NAME)

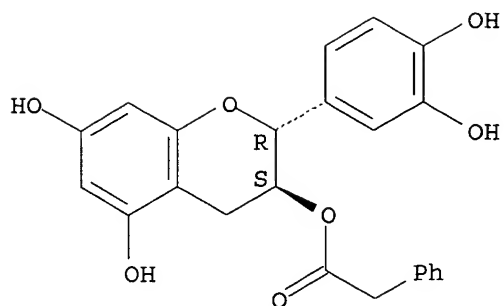
Absolute stereochemistry.



RN 71627-91-3 HCAPLUS

CN Benzeneacetic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-
dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 71627-94-6 HCAPLUS

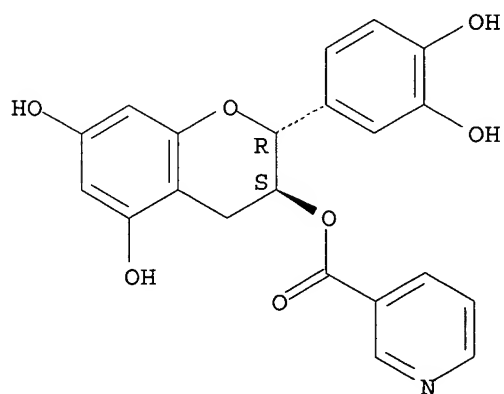
CN 3-Pyridinecarboxylic acid, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester, (2R-trans)-, trifluoromethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 71627-93-5

CMF C21 H17 N O7

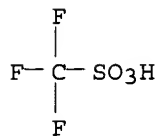
Absolute stereochemistry.



CM 2

CRN 1493-13-6

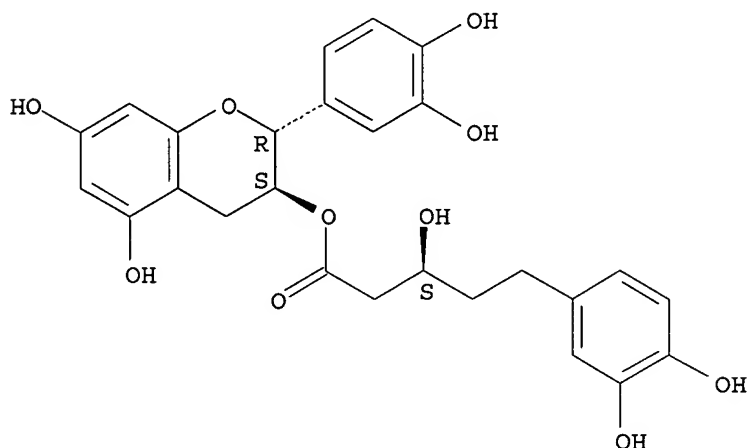
CMF C H F3 O3 S



=> d 150 ibib ab hitstr 1-10 100-110 179-189

L50 ANSWER 1 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:426215 HCAPLUS
DOCUMENT NUMBER: 140:209
TITLE: In vitro antileishmanial activity of proanthocyanidins and related compounds
AUTHOR(S): Kolodziej, Herbert; Kayser, O.; Kiderlen, A. F.; Ito, H.; Hatano, T.; Yoshida, T.; Foo, L. Y.
CORPORATE SOURCE: Institut fuer Pharmazie, Pharmazeutische Biologie, Freie Universitaet Berlin, Berlin, D-14195, Germany
SOURCE: Biodiversity: Biomolecular Aspects of Biodiversity and Innovative Utilization, [Proceedings of the IUPAC International Conference on Biodiversity], 3rd, Antalya, Turkey, Nov. 3-8, 2001 (2002), Meeting Date 2001, 265-268. Editor(s): Sener, Bilge. Kluwer Academic/Plenum Publishers: New York, N. Y.
CODEN: 69DZHW; ISBN: 0-306-47477-8
DOCUMENT TYPE: Conference
LANGUAGE: English
AB In vitro antileishmanial activity of proanthocyanidins and related compds. are discussed here.
IT 98570-83-3, Phylloflavan
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antileishmanial activity of proanthocyanidins and related compds.)
RN 98570-83-3 HCAPLUS
CN Benzenepentanoic acid, β ,3,4-trihydroxy-, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 2 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:123535 HCAPLUS
DOCUMENT NUMBER: 139:100023
TITLE: Extraction of tea catechins for chemicals analysis
AUTHOR(S): Horie, Hideki; Maeda-Yamamoto, Mari; Ujihara, Tomomi; Kohata, Katsunori

CORPORATE SOURCE: National Institute of Vergetable and Tea Science,
National Agricultural Research Organization, Shizuoka,
428-8501, Japan

SOURCE: Chagyo Kenkyu Hokoku (2002), 94, 60-64
CODEN: CHKHB9; ISSN: 0366-6190

PUBLISHER: Nippon Chagyo Gijutsu Kyokai

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

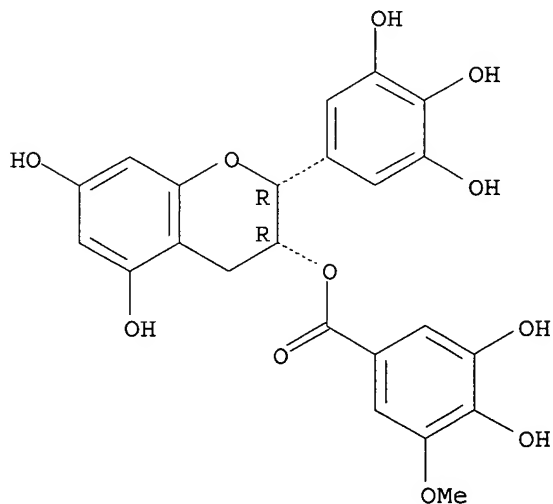
AB The efficient and safe methods were investigated to extract catechins,
strictinin and caffeine from tea leaves. The highest extraction rate was
achieved using the following method; (1) powdered tea leaves were suspended
in 2% aqueous solution of phosphoric acid, (2) the same volume of ethanol was
added
to the suspension, (3) the suspension was incubated at 30° for more
than 40 min.

IT 83104-87-4
RL: ANT (Analyte); ANST (Analytical study)
(extraction of tea catechins for chems. anal.)

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-
2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX
NAME)

Absolute stereochemistry. Rotation (-).



L50 ANSWER 3 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:668666 HCAPLUS

DOCUMENT NUMBER: 138:265441

TITLE: Suppression of cytotoxin-induced cell death in
isolated hepatocytes by tea catechins

AUTHOR(S): Kagaya, Noritaka; Tagawa, Yoh-ichi; Nagashima,
Hitoshi; Saijo, Ryoyasu; Kawase, Masaya; Yagi,
Kiyohito

CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, Osaka
University, Suita, Osaka, 565-0871, Japan

SOURCE: European Journal of Pharmacology (2002), 450(3),
231-236
CODEN: EJPHAZ; ISSN: 0014-2999

PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To elucidate the hepatoprotective effects of green tea catechins, the following expts. were conducted utilizing (-)-epigallocatechin-3-gallate (EGCG), the major component of green tea catechin, together with other catechins. The protective effects of catechins against hepatotoxins, bromobenzene or rubratoxin B, were examined in primary cultures of rat hepatocytes. Bromobenzene and rubratoxin B are known to induce necrosis and apoptosis of cells, resp. After 24-h treatment with toxin, EGCG and (-)-epigallocatechin-3-(3''-O-methyl)gallate (EGCg-3''-OMe) suppressed the bromobenzene-induced morphol. change and dose-dependently prevented bromobenzene-induced cell death. Both catechins also prevented apoptotic cell death caused by rubratoxin B. In rubratoxin B-treated cells, both catechins were found to suppress the activation of caspase-3 by rubratoxin B. The results in the present study suggest that EGCG and EGCg-3''-OMe are potent hepatoprotective agents. This report is the first to show that catechins suppress cytotoxin-induced cell death.

IT 83104-87-4

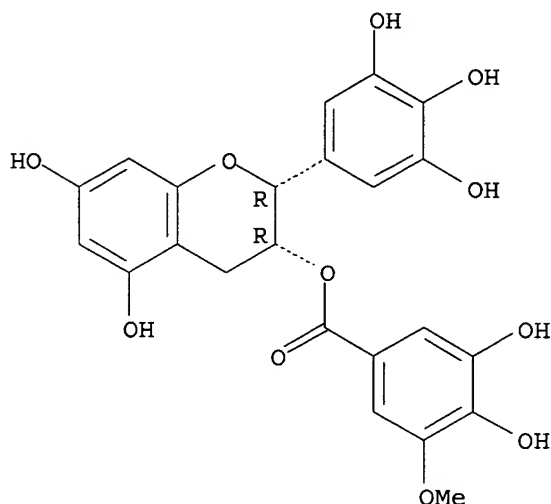
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(suppression of cytotoxin-induced cell death in isolated hepatocytes by tea catechins)

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 4 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:655531 HCAPLUS

DOCUMENT NUMBER: 137:320150

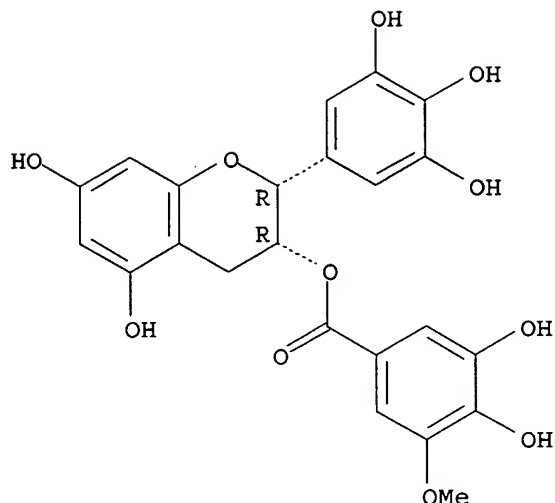
TITLE: Antiallergic Tea Catechin, (-)-Epigallocatechin-3-O-(3-O-methyl)-gallate, Suppresses Fc-ε-RI Expression in Human Basophilic KU812 Cells

AUTHOR(S): Fujimura, Yoshinori; Tachibana, Hirofumi;
Maeda-Yamamoto, Mari; Miyase, Toshio; Sano, Mitsuaki;
Yamada, Koji
CORPORATE SOURCE: Department of Bioscience and Biotechnology, Faculty of
Agriculture, Kyushu University, Higashi, Fukuoka,
812-8581, Japan
SOURCE: Journal of Agricultural and Food Chemistry (2002),
50(20), 5729-5734
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We previously found that the O-methylated derivative of (-)-epigallocatechin-3-O-gallate (EGCG), (-)-epigallocatechin-3-O-(3-O-methyl)-gallate (EGCG''3Me), has potent antiallergic activity. The high-affinity IgE receptor, Fc-ε-RI, is found at high levels on basophils and mast cells and plays a key role in a series of acute and chronic human allergic reactions. To understand the mechanism of action for the antiallergic EGCG''3Me, the effect of EGCG''3Me on the cell surface expression of Fc-ε-RI in human basophilic KU812 cells was examined. Flow cytometric anal. showed that EGCG''3Me was able to decrease the cell surface expression of Fc-ε-RI. Moreover, immunoblot anal. revealed that total cellular expression of the Fc-ε-RI α chain decreased upon treatment with EGCG''3Me. Fc-ε-RI is a tetrameric structure comprising one α chain, one β chain, and two γ chains. The level of mRNA production of each subunit in KU812 cells was investigated. EGCG''3Me reduced Fc-ε-RI α and γ mRNA levels. The cross-linkage of Fc-ε-RI causes the activation of basophils, which leads to the secretion of inflammatory mediators including histamine. EGCG''3Me treatment inhibited the Fc-ε-RI crosslinking-induced histamine release. These results suggested that EGCG''3Me can neg. regulate basophil activation through the suppression of Fc-ε-RI expression.

IT 83104-87-4, (-)-Epigallocatechin-3-O-(3-O-methyl) gallate
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(antiallergic tea catechin, epigallocatechin(methyl)gallate, suppresses
Fc-ε-RI expression in human basophilic KU812 cells)
RN 83104-87-4 HCAPLUS
CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-
2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX
NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 5 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:550974 HCAPLUS

DOCUMENT NUMBER: 138:117402

TITLE: Anti-allergic catechins of tea (*Camellia sinensis*)

AUTHOR(S): Maeda-Yamamoto, M.; Kawamoto, K.; Matsuda, N.; Sano, M.; Suzuki, N.; Yoshimura, M.; Tachibana, H.; Kawakami, Y.; Kawakami, T.; Hakamata, K.

CORPORATE SOURCE: National Research Institute of Vegetables, Ornamental Plants and Tea, Shizuoka, 428-8501, Japan

SOURCE: Animal Cell Technology: Basic & Applied Aspects, Proceedings of the Annual Meeting of the Japanese Association for Animal Cell Technology, 13th, Fukuoka and Karatsu, Japan, Nov. 16-21, 2000 (2002), Meeting Date 2000, 415-419. Editor(s): Shirahata, Sanetaka; Teruya, Kiichiro; Katakura, Yoshinori. Kluwer Academic Publishers: Dordrecht, Neth. CODEN: 69CWTU; ISBN: 1-4020-0271-8

DOCUMENT TYPE: Conference

LANGUAGE: English

AB Several in vitro and in vivo studies have demonstrated that components of tea (*Camellia Sinensis* L) exhibit biol. and pharmacol. properties. Antiallergic effect is one of these functional properties in which catechins apparently play a significant role. We report the anti-allergic effect of epigallocatechin-3-O-(3-O-methyl) gallate (EGCG3"Me) and epigallocatechin-3-O-(4-O-methyl) gallate (EGCG4"Me) isolated from Japanese (Assam hybrid) or Taiwanese tea leaves. Oral administration of these methylated catechins significantly and dose-dependently (5-50 mg/kg) inhibited type I allergic (anaphylactic) reactions in mice sensitized with ovalbumin and Freund's incomplete adjuvant. And these catechins strongly inhibited mast cell activation through the prevention of tyrosine phosphorylation (Lyn, Syk and Btk) of cellular protein and histamine/leukotrienes release, interleukin-2 secretion after Fcepsilon RI crosslinking. Furthermore, from the investigation that the effects of varieties, tea seasons of crops and manufacturing methods, to benefit the anti-allergic effect of EGCG3"Me, green or semi-fermented teas, made from Benihomare, Benifuuki and Benifuji at second crop onwards, should be

consumed.

IT 83104-87-4 224434-07-5

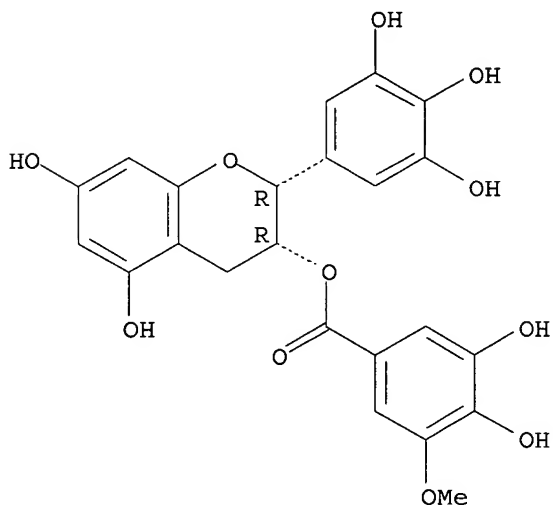
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)

(anti-allergic catechins of tea (*Camellia sinensis*))

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-
2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX
NAME)

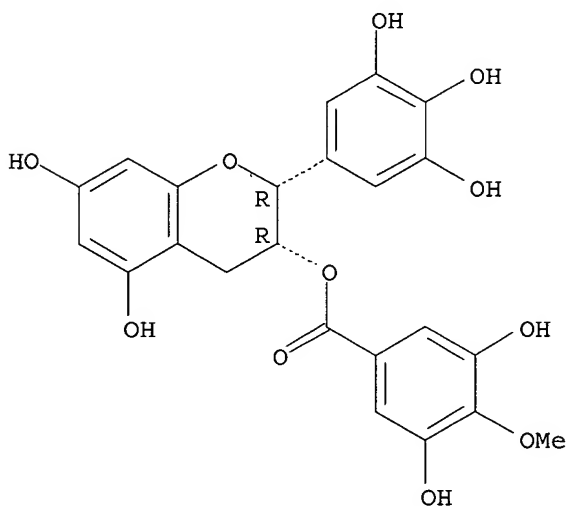
Absolute stereochemistry. Rotation (-).



RN 224434-07-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-
2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX
NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 6 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:481349 HCAPLUS

DOCUMENT NUMBER: 137:194955

TITLE: Identification and Characterization of Methylated and Ring-Fission Metabolites of Tea Catechins Formed in Humans, Mice, and Rats

AUTHOR(S): Meng, Xiaofeng; Sang, Shengmin; Zhu, Nanqun; Lu, Hong; Sheng, Shuqun; Lee, Mao-Jung; Ho, Chi-Tang; Yang, Chung S.

CORPORATE SOURCE: Laboratory for Cancer Research, College of Pharmacy, and Department of Chemistry, The State University of New Jersey, Piscataway, NJ, 08854, USA

SOURCE: Chemical Research in Toxicology (2002), 15(8), 1042-1050

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB (-)-Epigallocatechin gallate (EGCG), the most abundant tea catechin, has been proposed to be beneficial to human health based on its strong antioxidative and other biol. activities in vitro. Inadequate knowledge regarding the bioavailability and biotransformation of EGCG in humans, however, has limited our understanding of its possible beneficial health effects. In this study, 4',4''-di-O-methyl-EGCG (4',4''-DiMeEGCG) was detected in human plasma and urine by LC/MS/MS following green tea ingestion. Both 4',4''-DiMeEGCG and EGCG reached peak plasma values (20.5 ± 7.7 and 145.4 ± 31.6 nM, resp., in 4 subjects) at 2 h after the dose. The half-lives of 4',4''-DiMeEGCG and EGCG were 4.1 ± 0.8 and 2.7 ± 0.9 h, resp. The cumulative urinary excretion of 4',4''-DiMeEGCG during a 24 h period was 140.3 ± 48.6 μ g, about 5-fold higher than that of EGCG, but the excreted 4',4''-DiMeEGCG and EGCG in urine only accounted for about 0.1% of ingested EGCG. (-)-5-(3',4',5'-Trihydroxyphenyl)- γ -valerolactone (M4) and (-)-5-(3',4'-dihydroxyphenyl)- γ -valerolactone (M6), along with another possible ring-fission metabolite, (-)-5-(3',5'-dihydroxyphenyl)- γ -valerolactone (M6'), were detected in human urine after green tea ingestion. The cumulative excretion of M4, M6', and M6 during a 24 h period ranged from 75 μ g to 1.2 mg, 0.6 to 6 mg, and 0.6 to 10 mg, resp. The combined excretion of all three ring-fission metabolites accounted for 1.5-16% of ingested catechins. M4, M6', and M6 were all observed after the ingestion of pure EGCG or EGC by human subjects, whereas only M6 was produced after EC ingestion. These metabolites as well as monomethylated EGCG were detected in mice and rats after tea or EGCG administration, and the tissue levels reflected the rather low bioavailability of EGCG in rats. The presently characterized methylated EGCG metabolites and ring-fission products exist in substantial quantities and may contribute to the biol. activities of tea.

IT 224434-07-5P 298700-58-0P 452338-26-0P

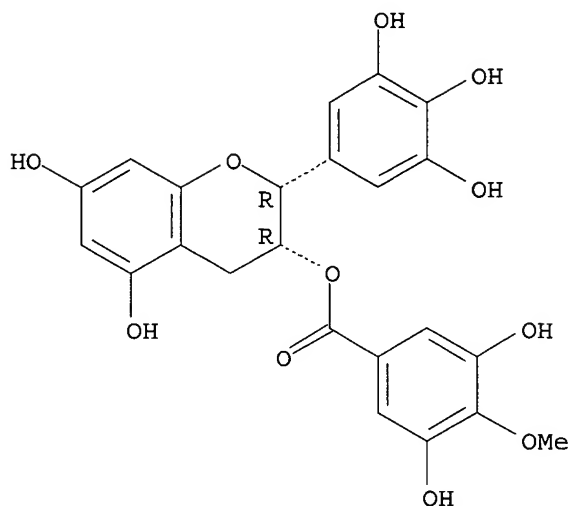
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(identification and characterization of methylated and ring-fission metabolites of tea catechins in humans, mice, and rats)

RN 224434-07-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

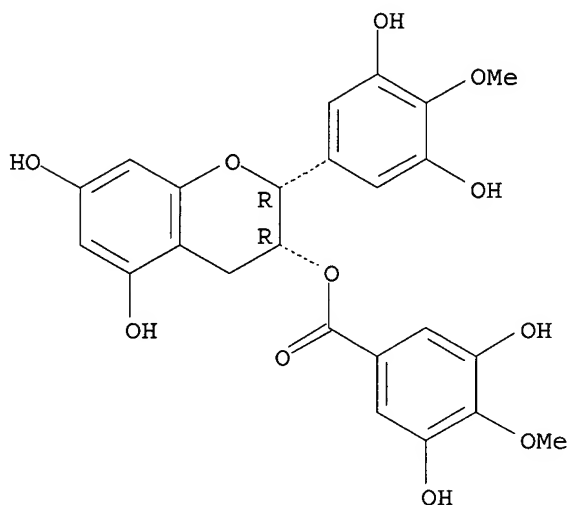
Absolute stereochemistry. Rotation (-).



RN 298700-58-0 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-2-(3,5-dihydroxy-4-methoxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI)
(CA INDEX NAME)

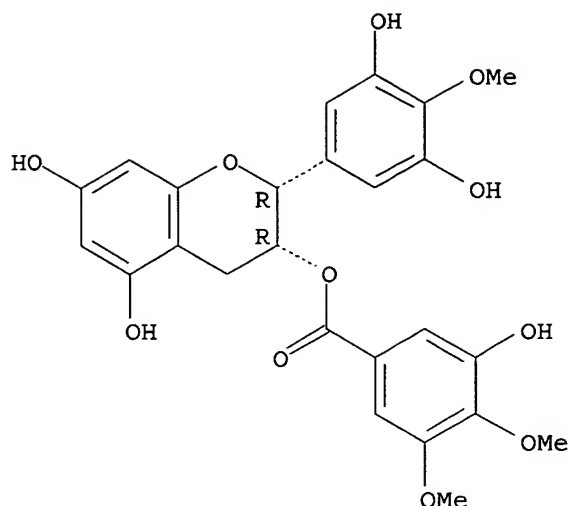
Absolute stereochemistry.



RN 452338-26-0 HCAPLUS

CN Benzoic acid, 3-hydroxy-4,5-dimethoxy-, (2R,3R)-2-(3,5-dihydroxy-4-methoxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 7 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:322415 HCAPLUS

DOCUMENT NUMBER: 137:351632

TITLE: Analysis for the biological functions of food factors using human cell lines

AUTHOR(S): Tachibana, Hirofumi

CORPORATE SOURCE: Graduate School of Agriculture, Kyushu University, Japan

SOURCE: Dojin News (2002), 102, 1-4
CODEN: DONEEA; ISSN: 0385-1516

PUBLISHER: Dojin Kagaku Kenkyusho

DOCUMENT TYPE: Journal; General Review

LANGUAGE: Japanese

AB A review. Many functional food-derived factors that can modulate physiologic systems of our body (i.e. endocrine, nerve, and immunologic systems) have been clarified, and these factors have been applied to create "functional foods". With respect to immunologic modulation, close attention is paid to how to suppress allergy, and the screening of the anti- or pro-allergic factors in foodstuffs has been performed. Tea (*Camellia sinensis*), one of today's most popular beverages, contains various substances. A number of studies have shown that tea has a wide range of biologic effects. Therefore the authors focused on tea leaves as a promising source for effective anti-allergic agents. To search for molecules that are able to suppress IgE synthesis, degranulation and high affinity IgE receptor expression, we examined various substances purified from tea for their effects on these aspects. Here we describe the identification of anti-allergic molecules found in tea leaves by using human cultured cell lines.

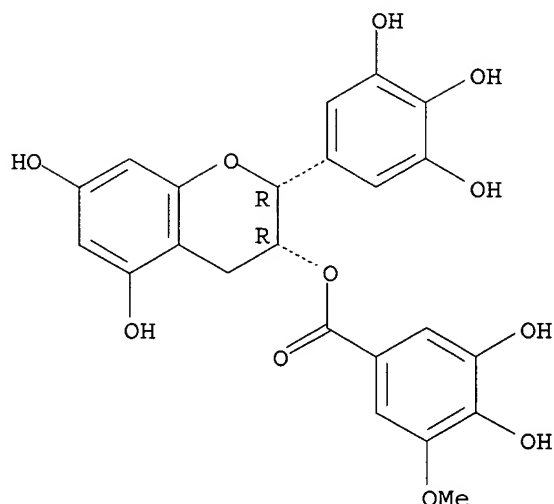
IT 83104-87-4

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anal. for antiallergy functions of green tea using human cell lines)

RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L50 ANSWER 8 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:251452 HCAPLUS

DOCUMENT NUMBER: 138:19107

TITLE: Structure-activity relationships for inhibition of human 5 α -reductases by polyphenols

AUTHOR(S): Hiipakka, Richard A.; Zhang, Han-Zhong; Dai, Wei; Dai, Qing; Liao, Shutsung

CORPORATE SOURCE: The Ben May Institute for Cancer Research, and The Tang Center for Herbal Medicine Research MC6027, Department of Biochemistry and Molecular Biology, University of Chicago, Chicago, IL, 60637, USA

SOURCE: Biochemical Pharmacology (2002), 63(6), 1165-1176
CODEN: BCPA6; ISSN: 0006-2952

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The enzyme steroid 5 α -reductase (EC 1.3.99.5) catalyzes the NADPH-dependent reduction of the double bond of a variety of 3-oxo- Δ 4 steroids including the conversion of testosterone to 5 α -dihydrotestosterone. In humans, 5 α -reductase activity is critical for certain aspects of male sexual differentiation, and may be involved in the development of benign prostatic hyperplasia, alopecia, hirsutism, and prostate cancer. Certain natural products contain components that are inhibitors of 5 α -reductase, such as the green tea catechin (-)-epigallocatechin gallate (EGCG). EGCG shows potent inhibition in cell-free but not in whole-cell assays of 5 α -reductase. Replacement of the gallate ester in EGCG with long-chain fatty acids produced potent 5 α -reductase inhibitors that were active in both cell-free and whole-cell assay systems. Other flavonoids that were potent inhibitors of the type 1 5 α -reductase include myricetin, quercetin, baicalein, and fisetin. Biochanin A, daidzein, genistein, and kaempferol were much better inhibitors of the type 2 than the type 1 isoenzyme. Several other natural and synthetic polyphenolic compds. were more effective inhibitors of the type 1 than the type 2 isoenzyme, including alizarin, anthrarobin, gossypol, nordihydroguaiaretic acid, caffeic acid phenethyl ester, and octyl and dodecyl gallates. The presence of a catechol group was

characteristic of almost all inhibitors that showed selectivity for the type 1 isoenzyme of 5 α -reductase. Since some of these compds. are consumed as part of the normal diet or in supplements, they have the potential to inhibit 5 α -reductase activity, which may be useful for the prevention or treatment of androgen-dependent disorders. However, these compds. also may adversely affect male sexual differentiation.

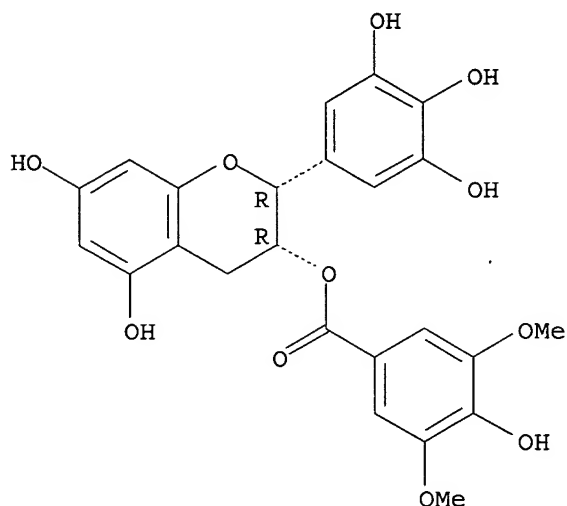
IT 173484-92-9 183209-70-3 224433-78-7
 224441-44-5 224441-50-3 224441-52-5
 224441-56-9 224441-58-1 224441-66-1
 224441-70-7

RL: PAC (Pharmacological activity); BIOL (Biological study)
 (structure-activity relationships for inhibition of human
 5 α -reductases by polyphenols)

RN 173484-92-9 HCAPLUS

CN Benzoic acid, 4-hydroxy-3,5-dimethoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-
 2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX
 NAME)

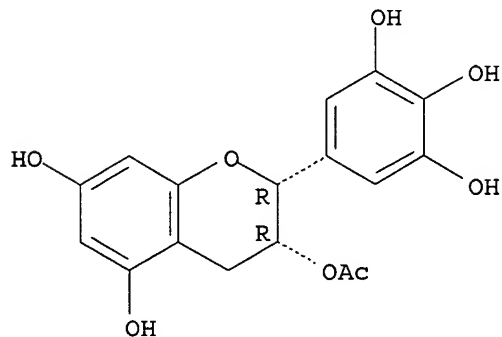
Absolute stereochemistry.



RN 183209-70-3 HCAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-,
 3-acetate, (2R,3R)- (9CI) (CA INDEX NAME)

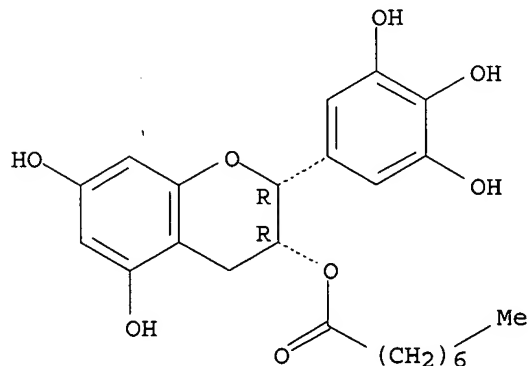
Absolute stereochemistry.



RN 224433-78-7 HCAPLUS

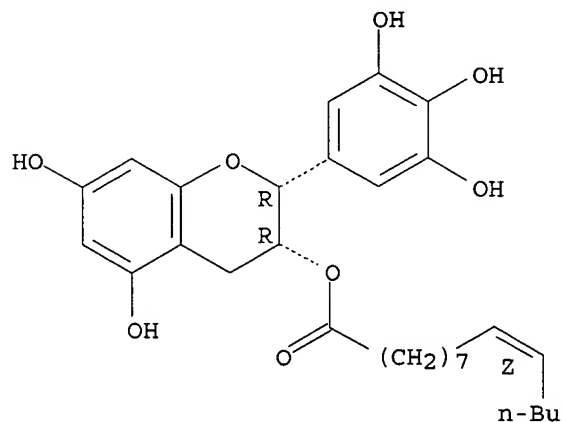
CN Octanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 224441-44-5 HCAPLUS

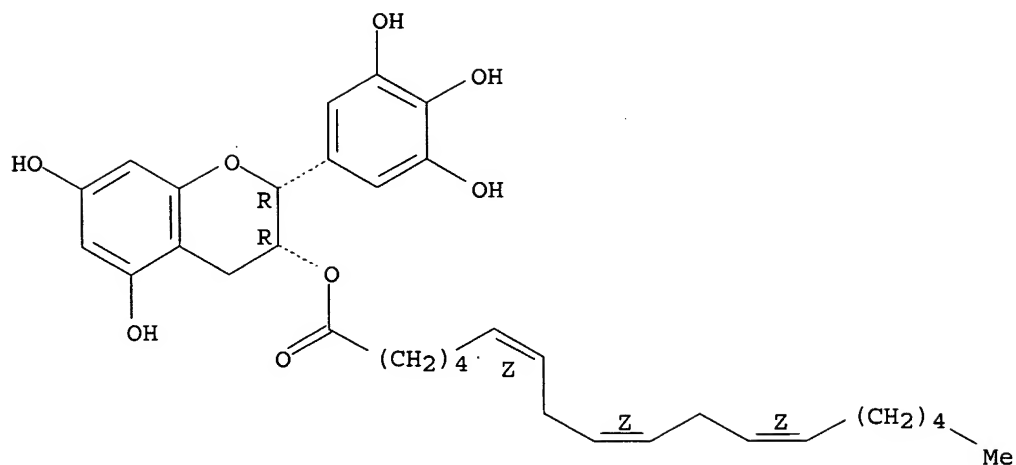
CN 9-Tetradecenoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, (9Z) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

RN 224441-50-3 HCAPLUS

CN 6,9,12-Octadecatrienoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, (6Z,9Z,12Z) - (9CI) (CA INDEX NAME)

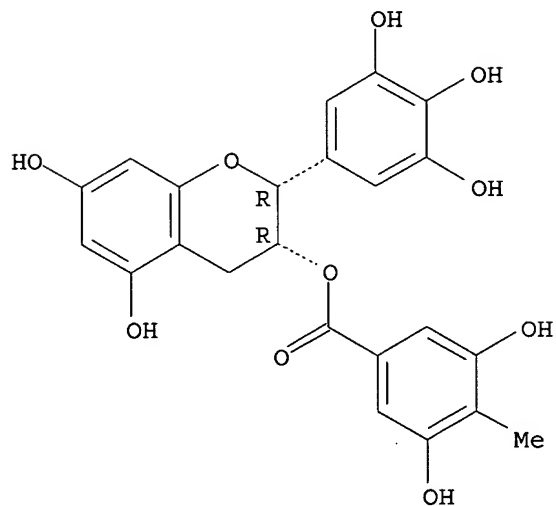
Absolute stereochemistry.
Double bond geometry as shown.



RN 224441-52-5 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methyl-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

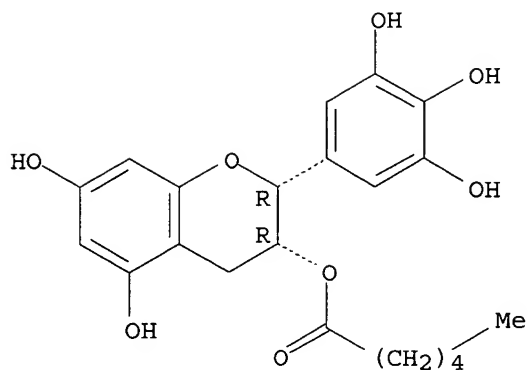
Absolute stereochemistry.



RN 224441-56-9 HCAPLUS

CN Hexanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

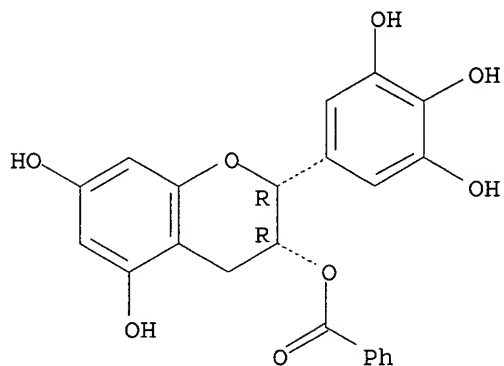
Absolute stereochemistry. Rotation (-).



RN 224441-58-1 HCAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, 3-benzoate, (2R,3R)- (9CI) (CA INDEX NAME)

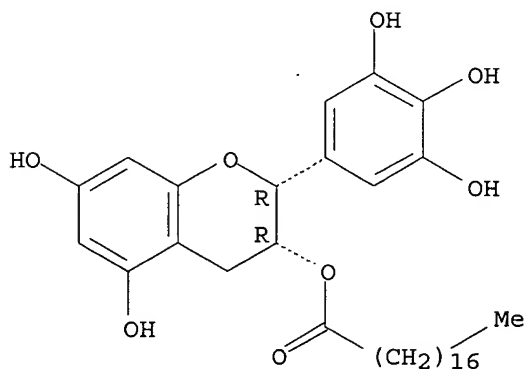
Absolute stereochemistry.



RN 224441-66-1 HCAPLUS

CN Octadecanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

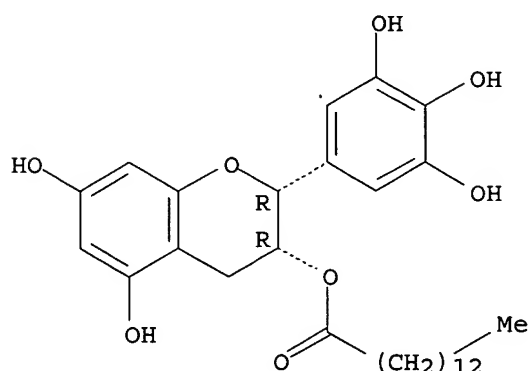


RN 224441-70-7 HCAPLUS

CN Tetradecanoic acid, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-

trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 9 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:173486 HCAPLUS

DOCUMENT NUMBER: 137:125009

TITLE: An efficient synthesis of the four mono methylated isomers of (+)-catechin including the major metabolites and of some dimethylated and trimethylated analogues through selective protection of the catechol ring

AUTHOR(S): Cren-Olive, Cecile; Lebrun, Stephane; Rolando, Christian

CORPORATE SOURCE: Chimie Organique et Macromoleculaire, Equipe Polyphenols, Universite des Sciences et Technologies de Lille, UPRESA 8009, Villeneuve d'Ascq, 59655, Fr.

SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2002), (6), 821-830

CODEN: JCSPCE; ISSN: 1472-7781

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:125009

AB The four monomethylated isomers of (+)-catechin (I) in positions 3', 4', 5 and 7, two dimethylated derivs., the 5,7-dimethylcatechin and the 3',4'-dimethylcatechin and two trimethylated isomers of (+)-catechin in positions 3', 5, 7 and 4', 5, 7 were synthesized by a new method based on successive and selective protections of the various phenol functions present on (+)-catechin. The key step was the selective protection of the catechol ring with dichlorodiphenylmethane and di-tert-butylidichlorosilane.

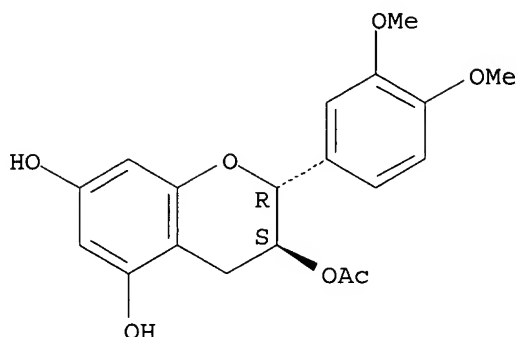
IT 443926-54-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of methylated isomers of (+)-catechin through selective protection of the catechol ring)

RN 443926-54-3 HCAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-, 3-acetate, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 96 THERE ARE 96 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 10 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:912018 HCAPLUS

DOCUMENT NUMBER: 136:385246

TITLE: Compositions and contents of catechins in various kinds of fresh tea leaves - comparisons between Assam variety and China variety-

AUTHOR(S): Saijo, Ryoyasu; Kato, Miyuki; Takeda, Yoshiyuki

CORPORATE SOURCE: Faculty of Education, Kagawa University, Kagawa, 760-8522, Japan

SOURCE: Special Publication - Royal Society of Chemistry (2001), 274 (Food Flavors and Chemistry), 183-196
CODEN: SROCD0; ISSN: 0260-6291

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Tea catechins, flavan-3-ol and flavan-3-gallate, are very important components showing astringency and bitterness of green and black teas. In addition orange and red color components of black tea infusion, i.e., theaflavins and thearubigins, are synthesized from those catechins during the fermentation process of the tea manufacture. The purpose of the present study is to make clear the composition and content of catechins contained in various kinds of fresh tea leaves from the Assam variety (*Camellia sinensis* var. *assamica*) and the China variety (*C. sinensis* var. *sinensis*). In the expts. 3 categories of tea leaves were used, i.e., young, mature and old leaves. Young fresh tea leaves consisting of a bud and three leaves were plucked in Apr., 1996 and 1997 in Makurazaki city, Kagoshima Prefecture. Catechin fraction was prepared from tea leaves by acetone extraction, Me iso-Bu ketone extraction and methanol dissoln. Ten naturally occurring catechins were analyzed by HPLC. The results obtained from fresh young tea leaves were: (-)-Epigallocatechin 3-gallate (EGCg), (-)-epicatechin 3-gallate (ECg), (-)-epigallocatechins (EGC) and (-)-epicatechin (EC) were the commonly present major catechins in tea leaves of all cultivars, accounting for 85.6 to 97.3% of the total catechins. On the other hand, (-)-epigallocatechin 3-(3"-O-methyl)gallate (EGCmetg), (-)-epicatechin 3-(3"-O-methyl)gallate (ECmetg), (-)-epigallocatechin 3,5-digallate (EGCgg), (-)-epicatechin 3,5-digallate (ECgg), (+)-gallocatechin (+G) and (+)-catechin (+C) were minor catechins in young tea leaves, accounting for the remaining 14.4 to 2.7%. EGCg was the major catechin in tea leaves, comprising 41.2 to 68.8% of the total catechins. The Assam variety

contained larger amts. of total catechins, EGCg, ECg, EGC, EGCgg and ECgg than the China variety. In contrast, the contents of EC were not much different between the Assam and the China varieties. EGCmetg and ECmetg were widely distributed in the Assam variety, the hybrids and the China variety. EGCgg and ECgg are likely to be characteristic components for the Assam variety. This is the 1st report to determine the contents of the 2 O-methylated gallates and the 2 digallates in tea leaves. The above characteristics were more prominent in young tea leaves than mature and old tea leaves.

IT 83104-86-3 83104-87-4

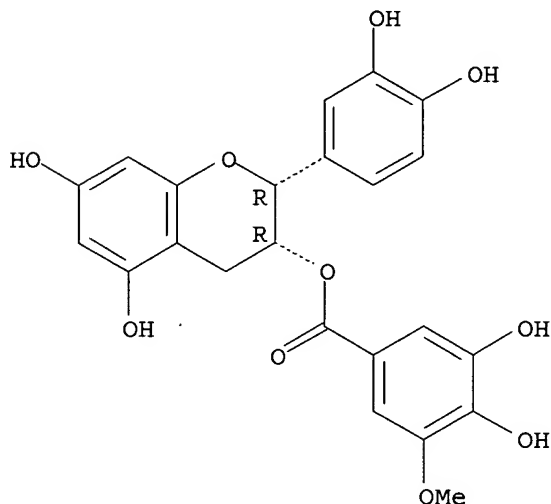
RL: ANT (Analyte); BSU (Biological study, unclassified); OCU (Occurrence, unclassified); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence)

(comps. and contents of catechins in various kinds of fresh tea leaves - comparisons between Assam variety and China variety)

RN 83104-86-3 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

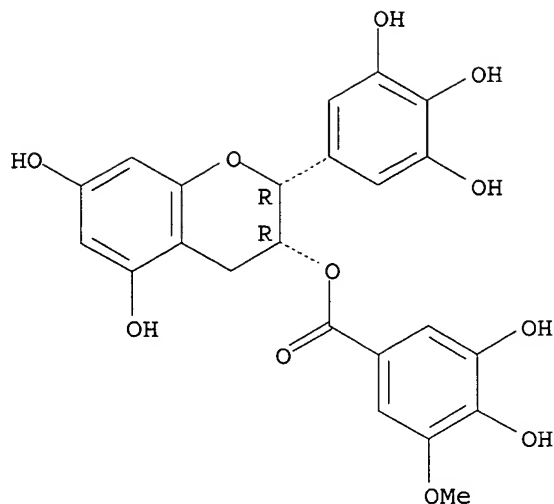
Absolute stereochemistry. Rotation (-).



RN 83104-87-4 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 100 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:507739 HCAPLUS

DOCUMENT NUMBER: 109:107739

TITLE: Flavans from *Crinum americanum*

AUTHOR(S): Ali, A. A.; Sayed, H. M.; Abdalla, O. M.; Steglich, W.

CORPORATE SOURCE: Fac. Pharm., Assiut Univ., Assiut, Egypt

SOURCE: Pharmazie (1988), 43(4), 295-6

CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:107739

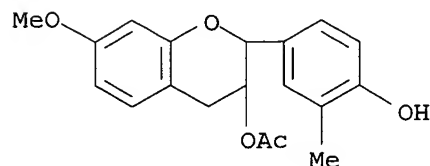
AB The isolation and characterization of 2 flavans from the chloroformic extract of defatted air-dried powdered bulbs of *Crinum americanum* is reported. The first compound, 4'-hydroxy-7-methoxy-5'-methylflavanol, is reported for the 1st time from plants, while the second, 4'-hydroxy-7-methoxyflavan has been previously identified in other plants. These compds. were identified by their phys. and chemical properties.

IT 116139-53-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 116139-53-8 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 3,4-dihydro-2-(4-hydroxy-3-methylphenyl)-7-methoxy-,
3-acetate (9CI) (CA INDEX NAME)



L50 ANSWER 101 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:470351 HCAPLUS

DOCUMENT NUMBER: 109:70351
TITLE: Tannins and related compounds. LXIII. Isolation and characterization of mongolicains A and B, novel tannins from Quercus and Castanopsis species
AUTHOR(S): Nonaka, Genichiro; Ishimaru, Kanji; Mihashi, Kunihide; Iwase, Yukiko; Ageta, Masayuki; Nishioka, Itsuo
CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(3), 857-69
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Continuing chemical exams. on tannins have led to the isolation of 2 new tannins, mongolicains A (I) and B (II), from 5 Quercus and 1 Castanopsis species. The structures of I and II have been characterized on the basis of chemical and spectroscopic data as novel flavanoellagitannins, in which hydrolyzable tannin and flavan-3-ol moieties are connected through a carbon-carbon linkage. Their structural features suggest that I and II are biosynthetically formed by oxidation of accompanying acutissimins A and B.
IT 115518-30-4P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
RN 115518-30-4 HCAPLUS
CN 9H,21H-29,19,21a-(Epoxyethanylylidene)-30,14,18-(epoxyethanylylidyne)-25H-dibenzo[7,8:9,10][1,5]dioxacycloundecino[3,2-c]pyrano[2',3':4,5]benzofuro[3,2-g][2]benzoxacyclooctadecin-5,9,21,32,38,41-hexone, 26-(acetyloxy)-27-(3,4-dimethoxyphenyl)-7,7a,26,27,28c,29,30,30a-octahydro-1,2,3,11,12,13,15,16,17,20,24,34,35,36-tetradecamethoxy- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L50 ANSWER 102 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:447849 HCAPLUS
DOCUMENT NUMBER: 109:47849
TITLE: Flavonoids as inhibitors of rat liver monooxygenase activities
AUTHOR(S): Beyeler, Suzy; Testa, Bernard; Perrissoud, Daniel
CORPORATE SOURCE: Sch. Pharm., Univ. Lausanne, Lausanne, CH-1005, Switz.
SOURCE: Biochemical Pharmacology (1988), 37(10), 1971-9
CODEN: BCPA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Flavanone (I) and 6 of its hydroxylated derivs., and cyanidanol (II) and 8 ethers and esters thereof, were investigated as inhibitors of cytochrome P 450-mediated reactions in rat liver microsomes. The 50% inhibitory values towards aminopyrine N-demethylation varied over a 20-fold range and depended on the pattern of hydroxylation (flavone derivs.) and on lipophilicity (cyanidanol derivs.). In the latter case, a bilinear relationship existed, the optimal log of the partition coefficient being 2.92. With selected compds., inhibitory concns. and Km and Vmax values were determined for aminopyrine N-demethylation, biphenyl 4-hydroxylation, and biphenyl 2-hydroxylation. Depending on the inhibitor and on the activity examined, noncompetitive, competitive, or mixed inhibition was seen. Interaction with cytochrome P 450 was also studied spectrally and was always found to result in a modified type II difference spectrum (ligand binding). A dual binding mode is postulated, involving electrostatic and lipophilic interactions.

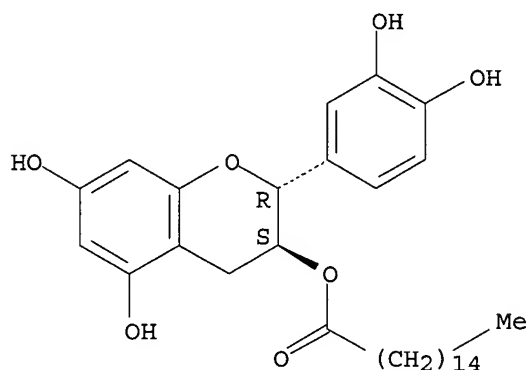
IT 71634-82-7 71634-84-9 71634-86-1

RL: BIOL (Biological study)
(cytochrome P 450-mediated monooxygenase of liver inhibition by,
structure in relation to)

RN 71634-82-7 HCAPLUS

CN Hexadecanoic acid, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

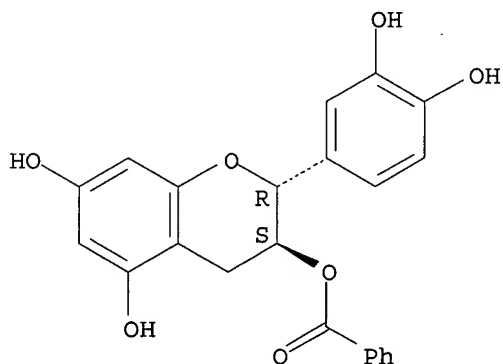
Absolute stereochemistry.



RN 71634-84-9 HCAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-,
3-benzoate, (2R-trans)- (9CI) (CA INDEX NAME)

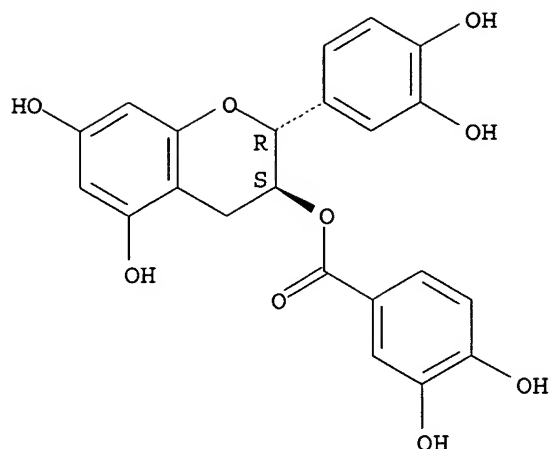
Absolute stereochemistry.



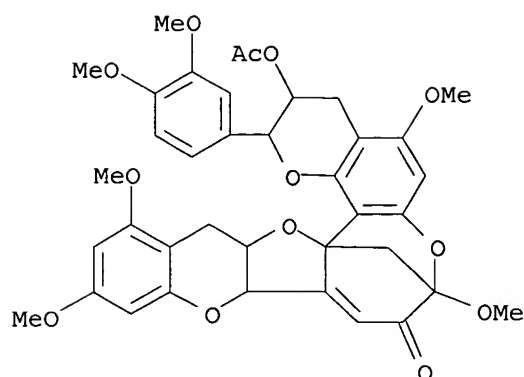
RN 71634-86-1 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester, (2R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 103 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1988:221433 HCAPLUS
 DOCUMENT NUMBER: 108:221433
 TITLE: Synthesis of condensed tannins. Part 19. Phenol oxidative coupling of (+)-catechin and (+)-mesquitol. Conformation of bis-(+)-catechins
 AUTHOR(S): Young, Desmond A.; Young, Esme; Roux, David G.; Brandt, E. Vincent; Ferreira, Daneel
 CORPORATE SOURCE: Dep. Chem., Univ. Orange Free State, Bloemfontein, 9300, S. Afr.
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (11), 2345-51
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:221433
 AB Oxidative coupling of (+)-catechin generates low yields of ether-([3'0,8]- and [4'08]-) and atropoisomeric C-linked ([2h,8]-, [2'6]-, and [6',8]-) bis-(+)-catechins. The isomeric structures were differentiated by NOE difference spectroscopy. Condensation of (+)-catechin with (+)-mesquitol readily affords the four atropoisomeric [5,6:5,8]-bis-[(+)-mesquitol]-(+)-catechins previously encountered in the heartwood of *Prosopis glandulosa* (Mesquite).
 IT **114580-72-2P**
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, by oxidative coupling of catechin)
 RN 114580-72-2 HCAPLUS
 CN 8,17a-Methano-2H,8H,17aH-[1]benzopyrano[2',3':4,5]furo[3,2-e]pyrano[2,3-h][1]benzoxocin-9(10bH)-one, 3-(acetyloxy)-2-(3,4-dimethoxyphenyl)-3,4,16,16a-tetrahydro-5,8,13,15-tetramethoxy-, [2R-(2 α ,3 β ,8a β ,10b α ,16a β ,17a α)]- (9CI) (CA INDEX NAME)



L50 ANSWER 104 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:183599 HCAPLUS

DOCUMENT NUMBER: 108:183599

TITLE: The structures of new biflavonoids from *Daphne odora* Thunb

AUTHOR(S): Baba, Kimiko; Takeuchi, Kazuo; Doi, Mitsunobu; Kozawa, Mitsugi

CORPORATE SOURCE: Osaka Univ. Pharm. Sci., Osaka, Japan

SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1987), 29, 668-75

CODEN: TYKYDS

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB The root and the bark of *D. odora* were examined in order to study its phenolics. Four new biflavonoids were isolated: daphnodorin A (I), daphnodorin B (II), daphnodorin C (III), and daphnodorin D (IV). The plane structures of I and II were established as furanoflavan type biflavonoid by chemical and spectral evidence. The absolute configurations of

I and II were assigned as C-2(S) and C-2(R), C-3(S) on the basis of their CD spectra and the x-ray anal. of a pentamethyl ether of I. The plane structure of III was determined to be spirobiflavonoid by chemical and spectral means. The absolute configuration of III was confirmed as C-2(S), C-2'(S) and C-3''(S) by chemical transformation of III into I and x-ray anal. of III. Compound IV was confirmed to be a mixture of atropisomers of flavan-8-3'' flavone by chemical and spectral evidence. Further, it was proved that III was transformed into I, IV, and a linear form of III in acidic or basic conditions. I, II, and III showed antimicrobial activity.

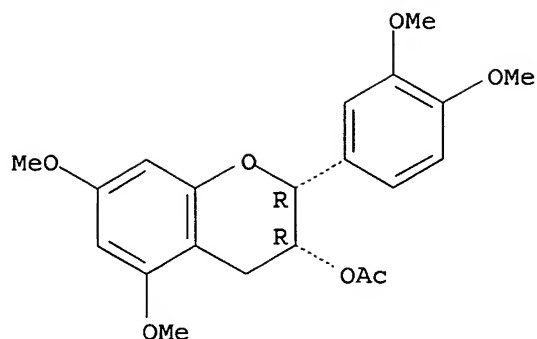
IT 58065-34-2P 58065-35-3P 95732-98-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 58065-34-2 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-5,7-dimethoxy-, acetate, (2R,3R)- (9CI) (CA INDEX NAME)

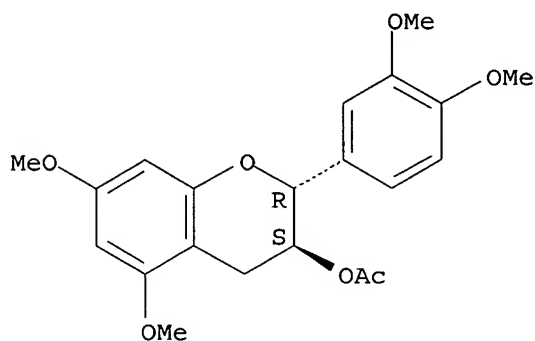
Absolute stereochemistry. Rotation (-).



RN 58065-35-3 HCAPLUS

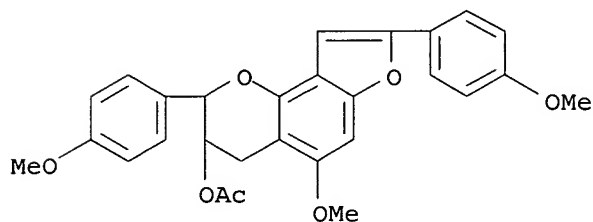
CN 2H-1-Benzopyran-3-ol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-5,7-dimethoxy-, acetate, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 95732-98-2 HCAPLUS

CN 2H-Furo[2,3-h]-1-benzopyran-3-ol, 3,4-dihydro-5-methoxy-2,8-bis(4-methoxyphenyl)-, acetate, (2R-trans)- (9CI) (CA INDEX NAME)



L50 ANSWER 105 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:128452 HCAPLUS

DOCUMENT NUMBER: 108:128452

TITLE: Phenylpropanoid derivatives of catechin, epicatechin and phylloflavan from Phyllocladus trichomanoides

AUTHOR(S): Foo, Lai Yeap

CORPORATE SOURCE: Chem. Div., DSIR, Petone, N. Z.

SOURCE: Phytochemistry (1987), 26(10), 2825-30

CODEN: PYTCAS; ISSN: 0031-9422

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Extraction of the cladodes of *P. trichomanoides* gave (+)-catechin, (-)-epicatechin, phylloflavan (I), and 2 phenylpropanoid derivative of epicatechin. In addition 3 novel compound identified as the phenylpropanoid derivs. of catechin (diastereomers, eg. II) and I (phylloflavanine, III) were isolated. The structures and configurations of these compound were established by chemical and spectroscopic evidence which led to a revised assignment of the configuration of the flavan unit in I.

IT 98570-83-3, Phylloflavan

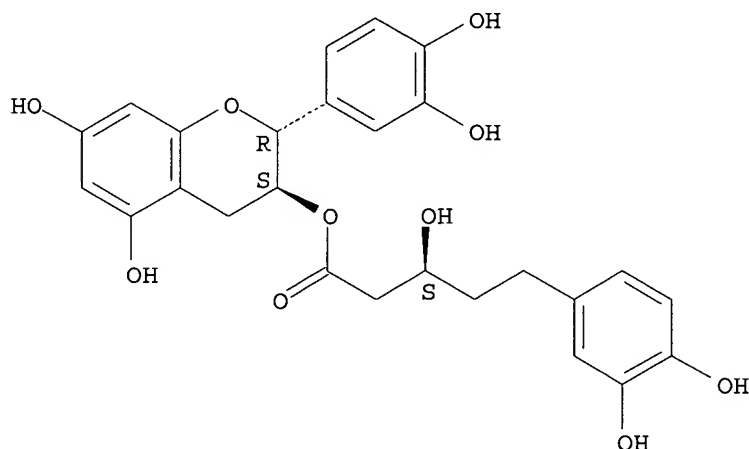
RL: BIOL (Biological study)

(from *Phyllocladus trichomanoides*, isolation and revision of the configuration of)

RN 98570-83-3 HCAPLUS

CN Benzenepentanoic acid, β ,3,4-trihydroxy-, (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 113296-20-1

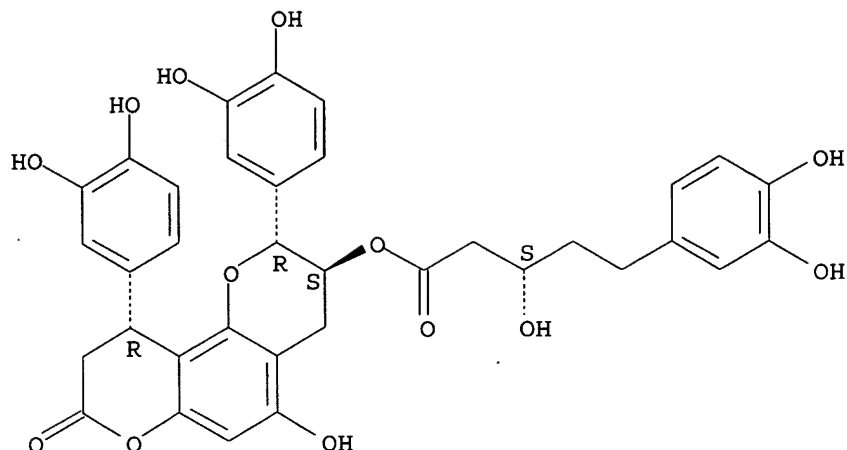
RL: BIOL (Biological study)

(from *Phyllocladus trichomanoides*)

RN 113296-20-1 HCAPLUS

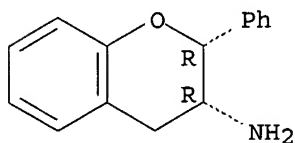
CN Benzenepentanoic acid, β ,3,4-trihydroxy-, (2R,3S,10R)-2,10-bis(3,4-dihydroxyphenyl)-3,4,9,10-tetrahydro-5-hydroxy-8-oxo-2H,8H-benzo[1,2-b:3,4-b']dipyrans-3-yl ester, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 106 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1988:55833 HCAPLUS
 DOCUMENT NUMBER: 108:55833
 TITLE: Reduction of α,β -unsaturated nitroalkenes with borane and borohydrides. A convenient route to 3-nitro-, 3-hydroxylamino-, and 3-amino-2H-1-benzopyran derivatives
 AUTHOR(S): Varma, Rajender S.; Gai, Yuan Zhu; Kabalka, George W.
 CORPORATE SOURCE: Dep. Chem., Univ. Tennessee, Knoxville, TN, 37996-1600, USA
 SOURCE: Journal of Heterocyclic Chemistry (1987), 24(3), 767-72
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:55833
 AB 3-Nitrochromenes were reduced by NaBH₄ in MeOH-THF to give chromans I [R₁ = H, Cl, NO₂; R₂ = H, OMe; R₃ = Ph, (EtO)₂C₆H₃, naphthyl]. Hydroxylamine analogs II [R₄ = Ph, Me₂CHC₆H₄, (EtO)₂C₆H₃, naphthyl] were obtained from nitrochromenes and BH₃-THF complex in THF containing NaBH₄.
 IT 112514-01-9P 112514-02-0P 112514-03-1P
 112514-04-2P 112514-06-4P 112514-07-5P
 112514-08-6P 112514-09-7P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 112514-01-9 HCAPLUS
 CN 2H-1-Benzopyran-3-amine, 3,4-dihydro-2-phenyl-, cis- (9CI) (CA INDEX NAME)

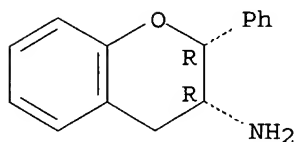
Relative stereochemistry.



RN 112514-02-0 HCAPLUS
 CN 2H-1-Benzopyran-3-amine, 3,4-dihydro-2-phenyl-, hydrochloride, cis- (9CI)

(CA INDEX NAME)

Relative stereochemistry.

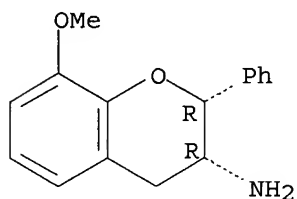


● HCl

RN 112514-03-1 HCAPLUS

CN 2H-1-Benzopyran-3-amine, 3,4-dihydro-8-methoxy-2-phenyl-, cis- (9CI) (CA INDEX NAME)

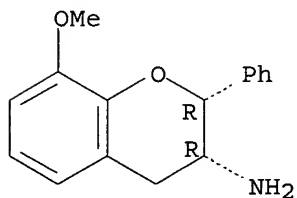
Relative stereochemistry.



RN 112514-04-2 HCAPLUS

CN 2H-1-Benzopyran-3-amine, 3,4-dihydro-8-methoxy-2-phenyl-, hydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

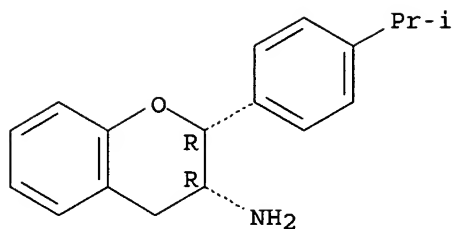


● HCl

RN 112514-06-4 HCAPLUS

CN 2H-1-Benzopyran-3-amine, 3,4-dihydro-2-[4-(1-methylethyl)phenyl]-, cis- (9CI) (CA INDEX NAME)

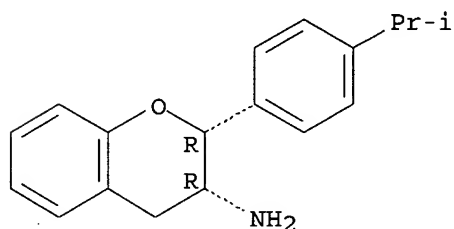
Relative stereochemistry.



RN 112514-07-5 HCAPLUS

CN 2H-1-Benzopyran-3-amine, 3,4-dihydro-2-[4-(1-methylethyl)phenyl]-, hydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

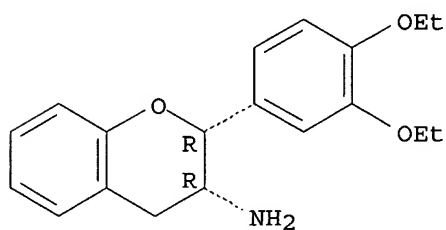


● HCl

RN 112514-08-6 HCAPLUS

CN 2H-1-Benzopyran-3-amine, 2-(3,4-diethoxyphenyl)-3,4-dihydro-, cis- (9CI) (CA INDEX NAME)

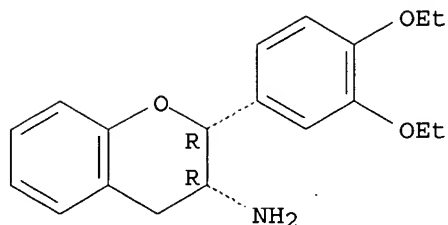
Relative stereochemistry.



RN 112514-09-7 HCAPLUS

CN 2H-1-Benzopyran-3-amine, 2-(3,4-diethoxyphenyl)-3,4-dihydro-, hydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

L50 ANSWER 107 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:34796 HCAPLUS

DOCUMENT NUMBER: 108:34796

TITLE: Novel flavonoids from the fern *Notholaena sulphurea*

AUTHOR(S): Arriaga-Giner, F. J.; Iinuma, M.; Tanaka, T.; Mizuno, M.; Scheele, C.; Wollenweber, E.

CORPORATE SOURCE: Dep. Quim. Org., Univ. Auton. Madrid, Madrid, E-28049, Spain

SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1987), 42(9-10), 1063-9

CODEN: ZNCBDA; ISSN: 0341-0382

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The major constituent of the yellow frond exudate of the fern *N. sulphurea* was identified by spectroscopic methods as 3,5,5'-trihydroxy-7-methoxy-8-acetoxyflavone and its structure was confirmed by synthesis. This novel natural flavonoid was also detected in the frond exudate of five other *Notholaena* species. In the yellow form of *N. sulphurea*, the rare 5,2'-dihydroxy-7,8-dimethoxyflavone was also found, along with some trivial flavonoids. The white form of *N. sulphurea* produces three dihydrochalcones that are accompanied by some kaempferol Me ethers and apigenin-7-Me ether. The 3-acetoxy as well as the 3-butyroxy and the 4'-butyroxy derivs. of 7-methylaromadendrin were also identified in this material. One of them belongs to the extremely rare group of 3-cis-dehydroflavonols.

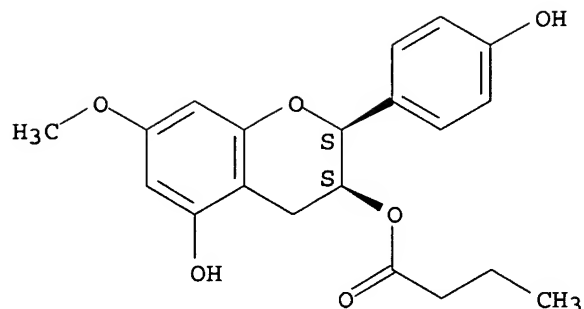
IT **112161-49-6P 112161-51-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 112161-49-6 HCAPLUS

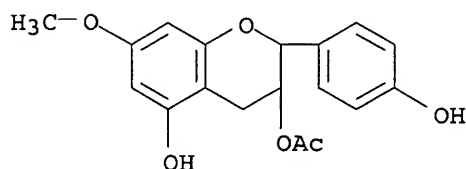
CN Butanoic acid, 3,4-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-2H-1-benzopyran-3-yl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry. .



RN 112161-51-0 HCAPLUS

CN 2H-1-Benzopyran-3,5-diol, 3,4-dihydro-2-(4-hydroxyphenyl)-7-methoxy-, 3-acetate (9CI) (CA INDEX NAME)



L50 ANSWER 108 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:554106 HCAPLUS

DOCUMENT NUMBER: 107:154106

TITLE: Synthesis of condensed tannins. Part 17. Oligomeric (2R,3S)-3,3',4',7,8-pentahydroxyflavans. Atropisomerism and conformation of biphenyl and m-terphenyl analogs from *Prosopis glandulosa* ('mesquite')

AUTHOR(S): Young, Esme; Brandt, Edward V.; Young, Desmond A.; Ferreira, Daneel; Roux, David G.

CORPORATE SOURCE: Dep. Chem., Univ. Orange Free State, Bloemfontein, 9300, S. Afr.

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1986), (10), 1737-49
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:154106

AB (2R,3S)-2,3-trans-3',4',7,8-Tetrahydroxyflavan-3-ol [(+)-mesquitol] (I), the predominant metabolite in the heartwood of *Prosopis glandulosa*, represents a putative precursor of a variety of oligomers, including conventional [4,6]- and [4,8]-biflavan-3-ols, a [1,6]-1,3-diarylpropylflavan-3-ol, [5,6]- and atropisomeric [5,8]-biphenyl-type biflavan-3-ols, and [5,6:5,8]-m-terphenyl-type triflavan-3-ols. Other participants in these condensations are mainly (+)-catechin, and also the flavan-3,4-diol analog of (+)-mesquitol. Oligomeric structures were confirmed by biomimetic oxidative and acid-induced couplings, and by nuclear Overhauser effect difference spectroscopy. These applications enabled correction of previous structural assignments for atropisomeric [5,8]-(+)-mesquitol-(+)-catechins and [5,6:5,8]-bis-[(+)-mesquitol]-(+)-catechins, and determination of their conformations.

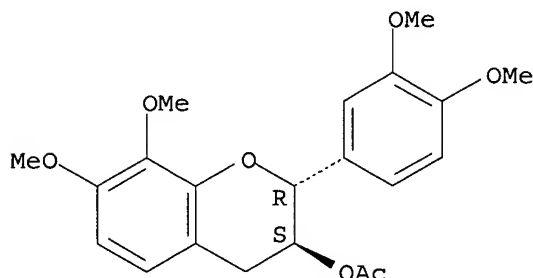
IT 109718-24-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 109718-24-3 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-7,8-dimethoxy-,
acetate, (2R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 109 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:438340 HCAPLUS

DOCUMENT NUMBER: 107:38340

TITLE: Tannins and related compounds. LVI. Isolation of
four new acylated flavan-3-ols from oolong tea. (1)
AUTHOR(S): Hashimoto, Fumio; Nonaka, Genichiro; Nishioka, Itsuo
CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1987), 35(2),
611-16

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A chemical examination of the aqueous acetone extract of com. oolong tea has
led to theisolation of four new acylated flavan-3-ols, together with known phenolic
comps. On the basis of chemical and spectroscopic evidence, the new comps.
have been characterized as (-)-epiafzelechin 3-O-gallate, (-)-epicatechin
3-O-(4-O-methyl)-gallate, (-)-epicatechin 3-O-p-hydroxybenzoate, and
(-)-epigallocatechin 3-O-cinnamate.

IT 83104-86-3 108907-44-4 108907-45-5

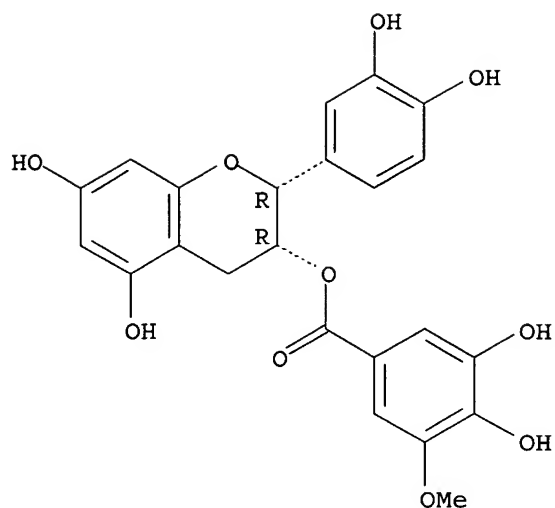
108907-46-6 110548-83-9

RL: BIOL (Biological study)
(from oolong tea, isolation and identification of)

RN 83104-86-3 HCAPLUS

CN Benzoic acid, 3,4-dihydroxy-5-methoxy-, (2R,3R)-2-(3,4-dihydroxyphenyl)-
3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX
NAME)

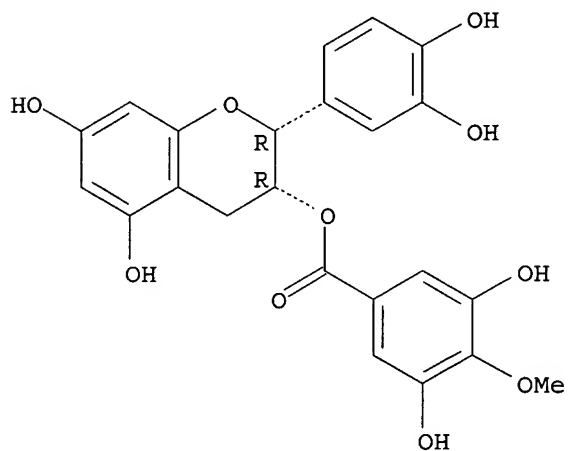
Absolute stereochemistry. Rotation (-).



RN 108907-44-4 HCAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-methoxy-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

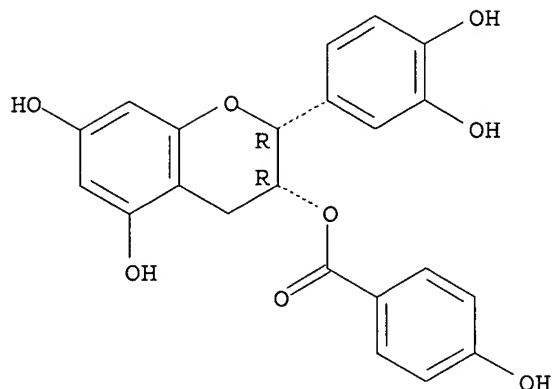
Absolute stereochemistry.



RN 108907-45-5 HCAPLUS

CN Benzoic acid, 4-hydroxy-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

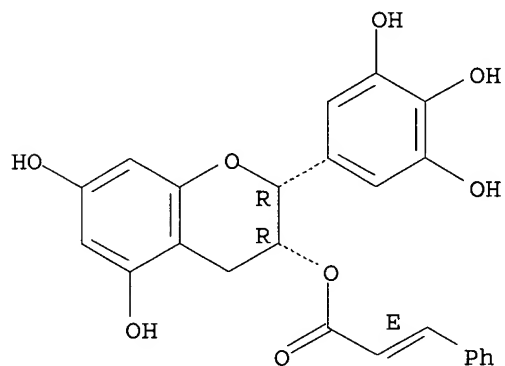
Absolute stereochemistry.



RN 108907-46-6 HCAPLUS

CN 2-Propenoic acid, 3-phenyl-, 3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, [2R-[2 α ,3 α (E)]]-(9CI) (CA INDEX NAME)

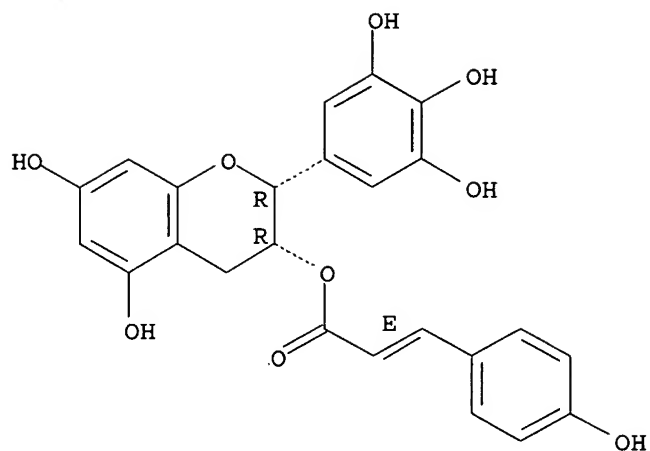
Absolute stereochemistry.
Double bond geometry as shown.



RN 110548-83-9 HCAPLUS

CN 2-Propenoic acid, 3-(4-hydroxyphenyl)-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester, (2E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



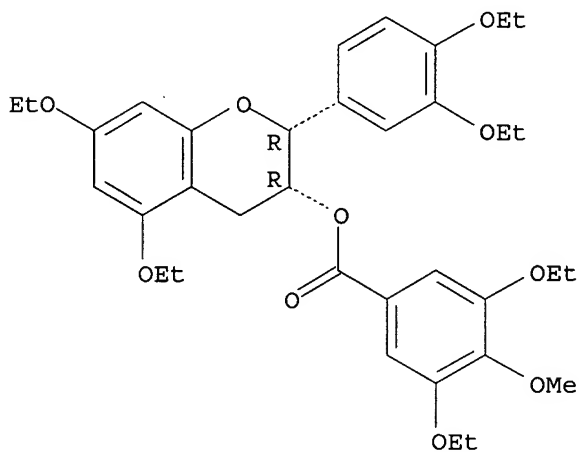
IT 108907-47-7P 108907-48-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 108907-47-7 HCAPLUS

CN Benzoic acid, 3,5-diethoxy-4-methoxy-, 2-(3,4-diethoxyphenyl)-5,7-diethoxy-3,4-dihydro-2H-1-benzopyran-3-yl ester, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

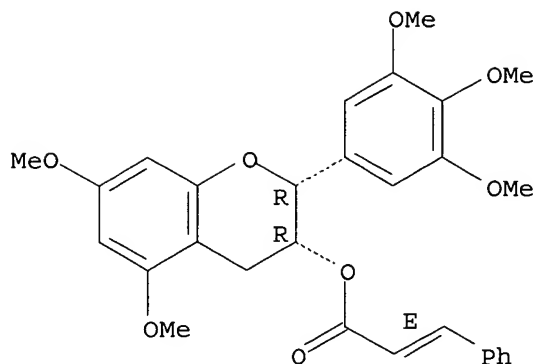


RN 108907-48-8 HCAPLUS

CN 2-Propenoic acid, 3-phenyl-, 3,4-dihydro-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-2H-1-benzopyran-3-yl ester, [2R-[2 α ,3 α (E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L50 ANSWER 110 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:49822 HCAPLUS

DOCUMENT NUMBER: 106:49822

TITLE: Chemical studies on the constituents of the thymelaeaceous plants. II. Stereochemistry of daphnodorin A and daphnodorin B

AUTHOR(S): Baba, Kimiye; Takeuchi, Kazuo; Doi, Mitsunobu; Inoue, Masatoshi; Kozawa, Mitsugi

CORPORATE SOURCE: Osaka Coll. Pharm., Matsubara, 580, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1986), 34(4), 1540-5

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

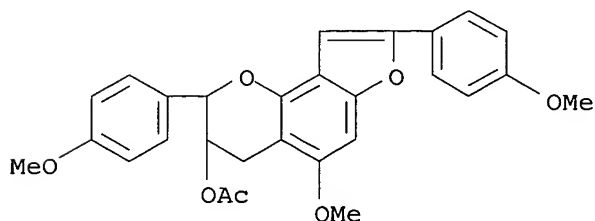
AB The absolute configurations of daphnodorin A [(S)-I, R = H] and daphnodorin B [(R,S)-I, R = OH] isolated from *Daphne odora* Thunb. (Thymelaeaceae) were assigned on the basis of chemical transformations and spectral analyses. An x-ray anal. of daphnodorin A pentamethyl ether was performed and 2 conformers were observed, due to restricted rotation of the trihydroxybenzoyl group.

IT 95732-98-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(CD of)

RN 95732-98-2 HCAPLUS

CN 2H-Furo[2,3-h]-1-benzopyran-3-ol, 3,4-dihydro-5-methoxy-2,8-bis(4-methoxyphenyl)-, acetate, (2R-trans)- (9CI) (CA INDEX NAME)



IT 58065-34-2 58065-35-3

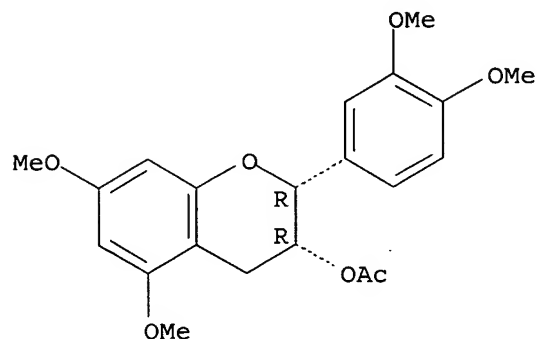
RL: RCT (Reactant); RACT (Reactant or reagent)
(NMR and CD of)

RN 58065-34-2 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-5,7-dimethoxy-,

acetate, (2R,3R)- (9CI) (CA INDEX NAME)

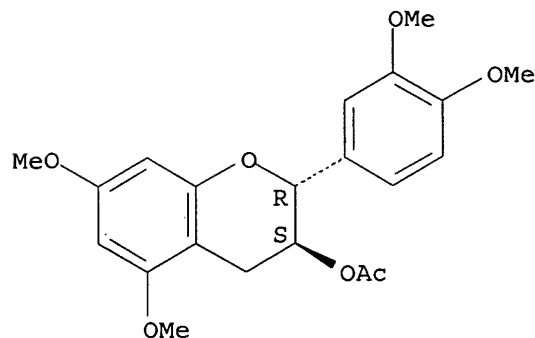
Absolute stereochemistry. Rotation (-).



RN 58065-35-3 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-5,7-dimethoxy-, acetate, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L50 ANSWER 179 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1962:416848 HCAPLUS

DOCUMENT NUMBER: 57:16848

ORIGINAL REFERENCE NO.: 57:3398a-c

TITLE: A new synthesis of flavans

AUTHOR(S): Keogh, E. J.; Philbin, Eva M.; Ushioda, S.; Wheeler, T. S.

CORPORATE SOURCE: Univ. Coll., Dublin, Ire.

SOURCE: Chemistry & Industry (London, United Kingdom) (1961) 2100-1

CODEN: CHINAG; ISSN: 0009-3068

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

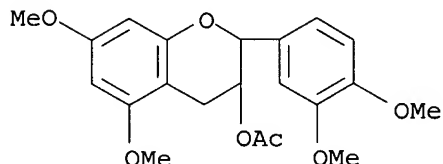
AB Reductive de sulfurization with Raney Ni in dioxane of thioketals (I) (X = ethylenedithio) gave the corresponding flavans (I, X = H₂) (II). The following compds. were used (R, R₁, R₂, R₃, m.p. I, and m.p. II given): H, H, H, H, 121°, 44-5°; H, OMe, H, H, 132°, 82°; OMe, OMe, OMe, OH, 177°, 145-7°; OMe, OMe, OMe, OAc, 154°, --; OMe, OMe, OMe, H, --, 110-11°.

IT 100735-99-7, 3-Flavanol, 3',4',5,7-tetramethoxy-, acetate

(preparation of)

RN 100735-99-7 HCAPLUS

CN 3-Flavanol, 3',4',5,7-tetramethoxy-, acetate (6CI, 7CI) (CA INDEX NAME)



L50 ANSWER 180 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1962:416847 HCAPLUS

DOCUMENT NUMBER: 57:16847

ORIGINAL REFERENCE NO.: 57:3396i,3397a-i,3398a

TITLE: Polymerization of flavans. VI. Reduction of flavanoids and chalcones with LiAlH₄ in the presence of AlCl₃

AUTHOR(S): Bokadia, M. M.; Brown, B. R.; Cobern, D.; Roberts, A.; Somerfield, G. A.

CORPORATE SOURCE: Univ. Oxford, UK

SOURCE: Journal of the Chemical Society, Abstracts (1962) 1658-66

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 57:16847

AB cf. CA 56, 11545g. The hydrogenolysis of flavan-4-one with a mixture of LiAlH₄ and AlCl₃ by a previously described method (CA 52, 4588d) gave 88% flavan (I), m. 43-4°, ν 752 and 697 cm.⁻¹ 4'-Methoxyflavan-4-one on reduction underwent ring cleavage and gave a 55% yield of o-HOC₆H₄CH₂CH₂CH₂C₆H₄MeO-p, isolated as its Bz derivative, m. 45.5-6.5°. The heterocyclic ether link of (+)epicatechin 5,7,3',4'-tetramethyl ether (II) was also hydrogenolyzed under these reduction conditions. Thus, 2 g. II added to a suspension of 0.5 g. LiAlH₄ and 3.5 g. AlCl₃ in 150 ml. tetrahydrofuran (THF), the mixture refluxed 6 hrs., decomposed at 0° with 10 ml. HCO₂Me in 50 ml. Et₂O and 20 ml. 2N H₂SO₄, the aqueous phase separated and extracted with Et₂O, the organic phase and exts.

combined and evaporated, the residue dissolved in 25 ml. 1:1 C₆H₆-Et₂O, the solution extracted with Claisen alkali, the phenolic material recovered from the

alkali extract and methylated (Me₂SO₄-Me₂CO-K₂CO₃), and the methylated product chromatographed on alumina yielded 140 mg. 2,4,6-

(MeO)₃C₆H₂CH₂CH(OH)CH₂C₆H₃(OMe)₂-3,4, m. 95-6.5° and 90 mg.

(+)-2,4,6-(MeO)₃C₆H₂CH₂CH(CH₂OH)C₆H₃(OMe)₂-3,4, m. 124.5-5.5°

(AcOEt-hexane), $[\alpha]_D$ 39.5° (1.1 g. CHCl₃). The

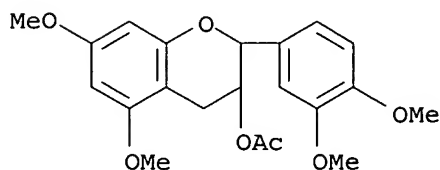
hydrogenolysis of γ,β -unsatd. ketones (chalcones) gave a variety of products. Thus, the reduction of chalcone with LiAlH₄ and AlCl₃ yielded 15% of a viscous oil (polymer?) and 65% trans-PhCH₂CH:CHPh, b_{0.15} 92°, n_D 1.5995, λ 204, 252, 284, and 292 m μ (ϵ 31600, 20600, 2500, and 2000, resp.), ν 963 cm.⁻¹ (trans-CH:CH); dibromide m. 110°. A similar reduction of p-MeOC₆H₄CH:CHCOPh gave 43% of a saturated polymer (?) and 44% of the isomeric olefin trans-p-MeOC₆H₄CH₂CH:CHPh (III), b_{0.01} 118°, n_D 1.5912, λ 254, 284, and 292 m μ (ϵ 14800, 4000, and 1300, resp.), ν 966 cm.⁻¹ (trans-CH:CH); dibromide m. 82-3°; bromo dibromide m.

130-2°. Likewise, p-MeOC₆H₄COCH:CHPh was reduced in 65% yield to the isomeric compound trans-p-MeOC₆H₄CH:CHCH₂Ph (IV), b_{0.15} 120-2°, n_D 1.5988, λ 257, 284, and 292 mμ (ε 28200, 5850, and 3200, resp.), ν 966 cm.⁻¹; dibromide m. 119-20° [with a reduction time of 20 min. a fraction containing some cis-olefin (ν 678 cm.⁻¹, characteristic of cis-CH:CH) also was obtained]. The course of the reaction was proposed as one of dehydration with double bond migration of an intermediate 1,3-diaryl-1-propanol, since the dehydration of p-MeOC₆H₄CH₂CH₂CH(OH)Ph and p-MeOC₆H₄CH(OH)CH₂CH₂Ph with AlCl₃ in Et₂O gave III and IV, resp. Further examples of these redns. were as follows: o-HOC₆H₄COCH:CHPh was isomerized on hydrogenolysis and gave 46% o-HOC₆H₄CH:CHCH₂Ph (V), m. 67-8°, λ 254 mμ (ε 26730), ν 3300 (OH), 970 (trans-CH:CH), 765, 740, and 690 cm.⁻¹ (aromatic); phenylurethan m. 138-9°. The reduction of o-HOC₆H₄COCH:CHC₆H₄OMe-p yielded 76% of the unisomerized product trans-o-HOC₆H₄CH₂CH:CHC₆H₄OMe-p (VI), m. 98.5-9.5°, λ 205, 262, 290 (inflection), and 310 mμ (inflection) (ε 37200, 28800, 4200, and 1900), ν 3580 (OH) and 972 cm.⁻¹ (trans-CH:CH), and 8% of the isomerized olefin trans-o-HOC₆H₄CH:CH-CH₂C₆H₄OMe-p (VII), m. 88-9°, λ 202, 260, and 300 mμ (inflection) (ε 32400, 25100, and 3900), ν 3413 (OH) and 975 cm.⁻¹. The structures of the reduction products of the 2'-hydroxychalcones were assigned from the ease of formation of flavans on treatment with acid. Thus, V boiled with Me-OH-HCl gave 15% I in 3 hrs. and 26% in 12 hrs., VI refluxed with EtOH-HCl for 2 hrs. under N gave 83% 4'-methoxyflavan (VIII), m. 83-4°, and VII refluxed with EtOH-HCl for 2 hrs. yielded no flavan derivative. The reduction of 11 g. o-HOC₆H₄CH:CHCOPh (IX) with 5 g. LiAlH₄ and 25 g. AlCl₃ in 150 ml. THF gave o-HOC₆H₄CH₂CH₂COPh, m. 90-1°, ν 3300 (OH) and 1670 cm.⁻¹ (aryl ketone) [Ac derivative (6.2 g.) m. 66-7°, ν 1760 (acetate) and 1690 cm.⁻¹ (aryl ketone)], and 2.2 g. o-HOC₆H₄CH₂CH₂CH(OH)Ph, m. 94.5-5.5°, λ 273 and 280 mμ (ε 2570 and 2220). Likewise, o-HOC₆H₄CH:CHCOC₆H₄OMe-p (X) on reduction yielded o-HOC₆H₄CH₂CH₂CH(OH)C₆H₄OMe-p m. 116.5-18°, o-HOC₆H₄CH₂CH₂COC₆H₄OMe-p, isolated as the Ac derivative, m. 83-4°, and a 30% yield of VIII. A 1-molar proportion IX refluxed for 30 min. in THF with a 4-molar proportion LiAlH₄ and a 20-25 mol. proportion AlCl₃ gave 17% I. The use of these increased proportions of LiAlH₄ and AlCl₃ afforded a 84% yield VIII and a 51% yield 3',4'-dimethoxyflavan from X and o-HOC₆H₄CH:CHCOC₆H₃(OMe)₂-3,4, resp. Other compds. reduced were as follows: (p-MeOC₆H₄CH₂)₂O (5.5 g.) was hydrogenolyzed to give 4.33 g. P-MeOC₆H₄Me. H₂C(OCH₂Ph)₂ (9.33 g.) on reduction gave 4.2 g. PhCH₂OMe and 2.9 g. PhCH₂OH; (PhCH₂)₂O was not reduced. Penicillium solitum grown on epimerized solns. of (+)-catechin gave II, m. 144-5° (MeOH), [α]_D 43° (3 g., CHCl₃); Ac derivative m. 93-5°, [α]_D 73° (2.4 g., CHCl₃).

IT 100735-99-7, 3-Flavanol, 3',4',5,7-tetramethoxy-, acetate (preparation of)

RN 100735-99-7 HCAPLUS

CN 3-Flavanol, 3',4',5,7-tetramethoxy-, acetate (6CI, 7CI) (CA INDEX NAME)



L50 ANSWER 181 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1962:53289 HCAPLUS

DOCUMENT NUMBER: 56:53289

ORIGINAL REFERENCE NO.: 56:10083a-i,10084a-d

TITLE: The absolute configuration of rotenone

AUTHOR(S): Buechi, G.; Crombie, L.; Godin, P. J.; Kaltenbronn, J. S.; Siddalingaiah, K. S.; Whiting, D. A.

CORPORATE SOURCE: Massachusetts Inst. of Technol., Cambridge

SOURCE: Journal of the Chemical Society, Abstracts (1961) 2843-60

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 56:53289

AB cf. Proc. Chemical Society 1960, 274. The configuration of natural rotenone (I)

was determined by exhaustive ozonolysis and oxidation as 5'-(R) and 6a-(S), and by

reduction of I and related compds. and obtaining of H-bonding indicated B/C cis-fusion, thus 12a-(S). Thus, I, m. 165-6° (CCl₄ and Cl₂CHCH₂Cl), polymorph m. 185-6°, [α]_{20D} -228° (c 2, 22, C₆H₆), was degraded to tubaic acid, m. 128.5-30.0° (Butenandt and Hildebrandt, CA 24, 1641), and this hydrogenated in EtOAc over Pd-BaSO₄ to give (-)-dihydrotubaic acid (II), m. 167-8°, [α]_{25D} -91° (CHCl₃). II (1.05 g.) in 50 mL. CHCl₃ was treated with 8 mg. O₃/min. at 0° for 3.5 h., decanted, evaporated, diluted with 25 mL. H₂O, refluxed 30 min., extracted continuously with Et₂O, and evaporated

to

give an oil (III), which slowly solidified. III was chromatographed on silica gel from C₆H₆ and eluted with C₆H₆-Et₂O to give a mixture of the hydroxy oxo acid and hydroxy acid. III (0.27 g.) in 10 mL. 4% KOH was treated with 4 mL. 30% H₂O₂ with cooling; after 1 h., the solution was warmed 15 min. at 50°, diluted with 20 mL. H₂O, acidified with SO₂, extracted with Et₂O, concentrated, chromatographed on silica gel, and eluted with 20:1 CHCl₃-Et₂O to give 0.154 g. (+)-3-hydroxy-4-methylpentanoic acid (IV), [α]_{25D} 26.4° (c 2.1, CHCl₃); 4-bromophenacyl ester m. 73.5-4.0°, [α]_{26D} 13.6° (c 0.74, CHCl₃). (±)-IV was prepared by treating BrCH₂CO₂CH₂Ph and Me₂CHCHO in C₆H₆Et₂O with Zn to give the ester, which was hydrogenolyzed and chromatographed to give (±)-IV; 4-bromophenacyl ester m. 83.5-4.0°. (±)-IV was resolved with quinine to give (-)-IV, [α]_{28D} -24.7° (c 0.98, CHCl₃); 4-bromophenacyl ester m. 74-5°, [α]_{25D} -14.4° (c 2, CHCl₃). (±)-IV (1.92 g.) was reduced with 0.76 g LiAlH₄ in 25 mL. Et₂O to give 1.26 g. (±)-4-methyl-1,3-pentanediol (V), b₁₀ 130° (bath); bis(α-naphthylcarbamate) m. 136-7°. Similarly prepared was (±)-V, n_{25D} 1.4482, [α]_{27D} -6.9° (c 2.84, CHCl₃). Crude V p-toluenesulfonate (1.47 g.) was reduced with 0.228 g. LiAlH₄ in 10 mL. Et₂O to give (±)-2-methyl-3-pentanol (VI), b₇₆₀ 135-40° (bath), n_{25D} 1.4173; 3,5-dinitrobenzoate (VII) m. 81-2°. Similarly prepared was (-)-VI, n_{25D} 1.4184, [α]_{27D} -8.5° (c 3.31, EtOH); 3,5-dinitrobenzoate, m. 89-92°, [α]_{26D} 4.9° (c 1.1, CHCl₃). Since (-)-IV was known to be correlated with L(-)-glyceraldehyde (VIII), (+)-IV from (-)-II was thus related to D-VIII and I had 5'(R) configuration. I (60 g.), 30 g. NaOAc, and 950 mL. Ac₂O refluxed 1 h., cooled, and poured into 1.6 l. H₂O gave 23 g. I enol acetate (IX), m. 162-4° (EtOH), [α]_{22D} -156° (c 2.05, C₆H₆); dimorph m. 136-7°. I (1 g.), 6 g. isopropenyl acetate, and 1 drop H₂SO₄ refluxed 15 min. gave IX, m. 164-5°

(EtOH). IX (20.6 g.) in 300 mL. Me₂CO hydrogenated over 2 g. 5% Pd-BaSO₄ gave 16.8 g. dihydro derivative (X) of IX, m. 208.5-10.5°, [α]_{26D} -161° (c 1.4, C₆H₆); (-)-dihydro derivative of I, isopropenyl acetate, and H₂SO₄ gave X in a second form, m. 174-5°, [α]_{20D} -164° (c 1.4, C₆H₆). X (5 g.) in 100 mL. 50% MeOH-CHCl₃ was ozonized at 0° 12 h., evaporated, refluxed with 50 mL. H₂O, evaporated, dissolved in MeOH-CHCl₃, ozonized, and treated as before to give 4.6 g. solid, which was chromatographed on an ion-exchange resin, eluted with N HOAc, and purified by the system of Palmer (CA 50, 9532h) to give 0.160 g. mixture of glyceric acid and IV. The mixture was converted to 4-bromophenacyl esters, crystallized from EtOH, then extracted with hexane to

leave

0.035 g. (-)-4-bromophenacyl glycerate, m. 109-111° (C₆H₆-hexane), [α]_{25D} -1.49° (c 4.36, acetone), which acid was known to be related to D-VIII, thus 6a-(S); hexane solubles gave 4-bromophenacyl ester of (+)-IV, m. 73.0-3.5°, [α]_{25D} 12.2° (c 2.31, CHCl₃), after chromatog. on alumina. (±)-Isorotenolone (XI) A and B Me ethers (Proc. Chemical Society 1960, 276) were each refluxed with concentrated HCl in

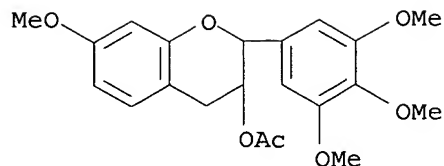
MeOH to

give 6a,12a-dehydroisorotenone (XII), m. 194-5°. (±)-XI A (0.4 g.), 2.5 mL. Ac₂O, 1 drop HOAc, and 2.5 g. Na₂SO₄ refluxed 15 min., diluted with MeOH, and poured into H₂O gave 0.16 g. XII; concentration of the filtrate gave 0.062 g. (±)-XI A acetate, m. 165°. Similarly, 0.25 g. (±)-XII B gave 0.12 g. XII and 0.0328 g. (±)-XII A acetate, m. 165°. (±)-XI A acetate was reduced with LiAlH₄ to (±)-iso A diol, m. 216°, which was the same as the reduction product of (±)-XI A and differed from either diol when (±)-XI B was treated similarly; the diol was the racemate and acetate of the cis series. (±)-Isorotenone with KBH₄ gave the 12α-hydroxy compound (XIII), m. 193° (CHCl₃-MeOH); 6a,-12a-XII with NaBH₄ gave XIII, which, when chromatographed from C₆H₆-CHCl₃ on alumina (activity I) gave the 12,12a-dehydro compound, m. 179°. Isorotenone (3 g.) in 50 mL. EtOAc hydrogenated at 100°/60 atmospheric over Pt catalyst, filtered, concentrated, and chromatographed from C₆H₆ on alumina gave 0.33 g. isorotenol, m. 131-2°, and 1.5 g. XIII, m. 195° (EtOH); the presence of H-bonding (0.5) indicated OH to be α. Hydrogenation of unsatd. derivs. of I containing cis-B/C fusion with cis addition were as follows. 6a,-12a-Dehydro derivative of I (9.5 g.) in 200 mL. EtOAc was hydrogenated over Pt catalyst at 25°/10 atmospheric for 36 h., filtered, and concentrated to give 3.5 g. 6a,12a-dehydro-6',7'-dihydro derivative (XIV) of I, m. 226-7°; the filtrate concentrated further gave a residue, which was extracted with 2% KOH and acidified, and the aqueous layer extracted with CHCl₃, to give 1',5'-seco compound, "dehydrodihydroisorotenonic acid," m. 221° (EtOH). XIV (2 g.) was hydrogenated over PtO₂ in EtOAc 7 days at 70°/60 atmospheric to give 1.5 g. 6',7'-dihydroisorotenol, m. 133° (EtOH). 6a,12a-Dehydro-α-toxicarol (1 g.), m. 230-1°, was hydrogenated in HOAc over PtO₂ at 75° until 125 mL. H was absorbed; the mixture filtered and chromatographed from CHCl₃ gave (±)-4',5'-dihydro-α-toxicarol (XV), m. 206°. (±)-α-Toxicarol was hydrogenated to give X m. 209-10°. Hydrogenolysis of other rotenoid derivs., such as (-)-4',5'-dihydrodeguelin, maintained the cis-B/C fusion configurations. Addnl. evidence of 12a-(S), cis-B/C fusion was given.

IT 100736-00-3, 3-Flavanol, 3',4',5',7-tetramethoxy-, acetate
(preparation of)

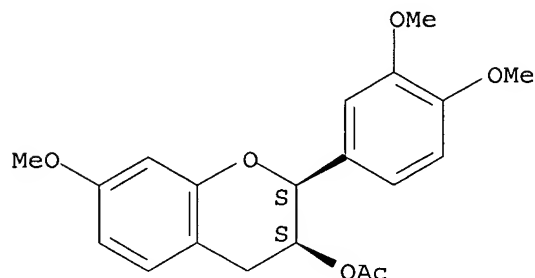
RN 100736-00-3 HCAPLUS

CN 3-Flavanol, 3',4',5',7-tetramethoxy-, acetate (6CI, 7CI) (CA INDEX NAME)



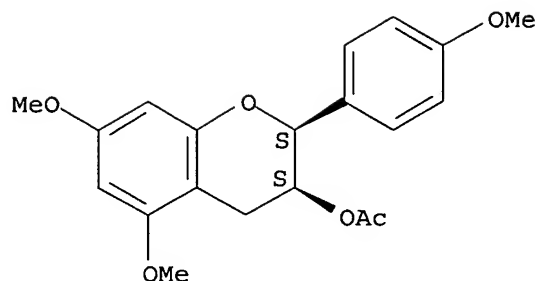
L50 ANSWER 182 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1962:53288 HCAPLUS
 DOCUMENT NUMBER: 56:53288
 ORIGINAL REFERENCE NO.: 56:10082h-i,10083a
 TITLE: A new method for the synthesis of cis-catechins
 AUTHOR(S): Kashikar, M. D.; Kulkarni, R. S.; Borkar, A. M.;
 Kulkarni, A. B.
 CORPORATE SOURCE: Inst. Sci., Bombay
 SOURCE: Chemistry & Industry (London, United Kingdom) (1961)
 1872
 CODEN: CHINAG; ISSN: 0009-3068
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Reduction of flavonol benzyl ether, m. 114-15°, with LiAlH₄ followed by
 hydrogenation of the complex in situ over Raney Ni gives catechin in
 better yields than are obtained when flavonol benzoate is reduced this way
 (CA 54, 17384f). Similarly, 4',5,7-trimethoxyflavonol benzyl ether, m.
 166°, was reduced to (±)-cis-afzelechin trimethyl ether, m.
 113-14° (acetate m. 127°); 3',4',7-trimethoxyflavonol benzyl
 ether, m. 113-14°, gave (±)-cis-fisetinidol trimethyl ether, m.
 156-8° (acetate m. 168-70°); 3',4',5',7-tetramethoxyflavonol
 benzyl ether, m. 125-7°, gave (±)-cis-robinetinidol tetramethyl
 ether, m. 150-2°; acetate m. 136-8°.
 IT 803-88-3, 3-Flavanol, 3',4',7-trimethoxy-, cis-, acetate
 804-02-4, 3-Flavanol, 4',5,7-trimethoxy-, cis-, acetate
 100736-00-3, 3-Flavanol, 3',4',5',7-tetramethoxy-, acetate
 (preparation of)
 RN 803-88-3 HCAPLUS
 CN 2H-1-Benzopyran-3-ol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-7-methoxy-,
 acetate, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

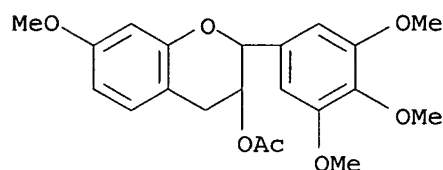


RN 804-02-4 HCAPLUS
 CN 3-Flavanol, 4',5,7-trimethoxy-, acetate, cis-(±)- (8CI) (CA INDEX
 NAME)

Relative stereochemistry.



RN 100736-00-3 HCAPLUS
 CN 3-Flavanol, 3',4',5',7-tetramethoxy-, acetate (6CI, 7CI) (CA INDEX NAME)



L50 ANSWER 183 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1961:48654 HCAPLUS

DOCUMENT NUMBER: 55:48654

ORIGINAL REFERENCE NO.: 55:9390a-d

TITLE: Condensed tannins. VII. Isolation of
 (-)-3',4',7-trihydroxyflavan-3-ol [(-)-fisetinidol], a
 naturally occurring catechin from black-wattle
 heartwood

AUTHOR(S): Roux, D. G.; Paulus, E.

CORPORATE SOURCE: Rhodes Univ., Grahamstown, S. Afr.

SOURCE: Biochemical Journal (1961), 78, 120-3

CODEN: BIJOAK; ISSN: 0264-6021

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. CA 55, 7554a. EtOAc-soluble compds. from black-wattle heartwood isolated
 as described (loc. cit.) were dissolved in EtOAc to which was added 1/2
 volume CHCl₃. The tannin precipitate was removed by filtration and the
 filtrate

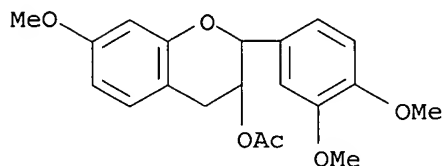
dried in vacuo. After extraction of the wax from the residue with ligroine,
 the material was treated by a countercurrent process to give (+)-fustin,
 leucofisetinidin, (+)-mollisaccacidin, and (-)-fistinidol (I), m.
 211-14°. I was converted to (-)-3',4',7-trimethoxyflavan-3-ol by
 treatment in MeOH with CH₂N₂ 24 hrs. at -5°, m. 121-23°, $[\alpha]_{25D} -31.9 \pm 0.6^\circ$ (C₂H₂Cl₄). The radial distribution of
 I was determined in 50 yr. old specimens of *Acacia mollissima*. I had the same
 configuration at C-2 and C-3 as (+)-3',4',7-trihydroxyflavan-3,4-diol and
 (+)-fustin. Flavan-3,4-diol may be the single precursor from which the
 corresponding catechin, 2,3-dihydroflavanol, and flavanol arise by
 inter-conversion, and the accompanying leucofisetinidin condensed tannins
 by condensation. I was synthesized from (+)-mollisaccacidin
 [(+)-3',4',7-trihydroxyflavan-3,4-diol] by hydrogenation according to the
 method of Weinges (Ann. 627, 229(1959); CA 53, 4264g). I was methylated
 in MeOH with CH₂N₂ yield tri-O-methyl-(-)-fisetinidol, m. 121-23°,

$[\alpha]_{23D} -32.1 \pm 0.7^\circ$ (C₂H₂Cl₄). Acetylation of this compound with C₅H₅N-Ac₂O 3 hrs. at room temperature yields O-acetyltri-O-methyl-(-)-fisetinidol, long needles, m. 95-7° (EtOH), $[\alpha]_{23D} -19.1 \pm 1.5^\circ$ (C₂H₂Cl₄). I was acetylated as above for 3 and 24 hrs. to yield tetra-O-acetyl-(-)-fisetinidol, m. 50-60°, $[\alpha]_{23D} 0.9 \pm 0.2^\circ$ (C₂H₂Cl₄).

IT 99950-73-9, 3-Flavanol, 3',4',7-trimethoxy-, acetate (preparation of)

RN 99950-73-9 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-7-methoxy-, acetate (9CI) (CA INDEX NAME)



L50 ANSWER 184 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1961:2659 HCAPLUS

DOCUMENT NUMBER: 55:2659

ORIGINAL REFERENCE NO.: 55:526h-i,527a-c

TITLE: The chemistry of eucalypt kinos. III. (+)-Afzelechin, pyrogallol, and (+)-catechin from Eucalyptus calophylla kino

AUTHOR(S): Hillis, W. E.; Carle, Ann

CORPORATE SOURCE: Div. Forest Products, C.S.I.R.O., Melbourne

SOURCE: Australian Journal of Chemistry (1960), 13, 390

CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. CA 47, 3305a. Two dimensional paper chromatography of the E. calophylla kino (I) with 6% HOAc followed by 6:1:2 BuOH-AcOH-H₂O disclosed, on examination under ultraviolet light before and after fuming with NH₃ and spraying with diazotized p-nitroaniline-NaOAc, vanillin-HCl and FeCl₃-K₃Fe(CN)₆, the presence of 21 compds. In addition to aromadendrin, kaempferol, and ellagic acid, previously identified by H. (CA 47, 3305a), catechin, epicatechin and galocatechin were also identified by cochromatography. Dry Et₂O extract (100 g.) of I was dissolved in 80 ml. MeOH and 600 ml. Et₂O and the mixture added to the first 5 tubes of a countercurrent distribution apparatus containing 150 ml. H₂O in each tube.

After

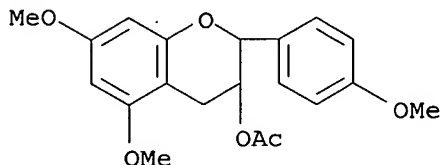
fractionation with Et₂O and chromatographic examination of the contents of the 72 tubes and 18 aliquots (A-H) discharged from the final tube, these were grouped, the groups extracted with Et₂O and EtOAc, and the exts. evaporated. Secondary fractionation of the extract from tubes 39-72 and aliquots R-H on a cellulose column with 6% AcOH led to isolation of 1.3 g. pyrogallol and 1.1 g. (+)-afzelechin (II), thin colorless needles, soluble in H₂O and organic solvents, m. 221-2° (decomposition), $[\alpha]_{20D} 20.6^\circ$ (c 5%, 1:1 Me₂CO-H₂O). Infrared spectrum (KCl disc) was determined; λ_{maximum} 214, 277 m μ , λ_{min} 255 m μ . II (0.3 g.) in 90 ml. Et₂O gave with CH₂N₂ in Et₂O 0.13 g. 5,7,4'-trimethoxy-3-flavanol (III), m. 134-5°, $[\alpha]_{20D} -0.9^\circ$ (2% C₂H₂Cl₄), -5.7° (2% EtOH); acetate prepared with Ac₂O-C₅H₅N, m. 88-90° (EtOH). Oxidation of III with KMnO₄ gave p-anisic acid. II in Ac₂O-C₅H₅N gave

3,5,7,4'-tetraacetoxyflavan, m. 109°. Data showed II to be 3,5,7,4'-tetrahydroxyflavan. Dry material from tubes 17-38 crystallized from H₂O had $[\alpha]_{20D} 16.1^\circ$ (1:1 Me₂CO: H₂O); pentaacetate m. 131°; 5,7,3',4'-tetra-Me ether m. 141°. Mixed m.p. with (+)-catechin was 174-5°.

IT 99950-71-7, 3-Flavanol, 4',5,7-trimethoxy-, acetate
(preparation of)

RN 99950-71-7 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 3,4-dihydro-5,7-dimethoxy-2-(4-methoxyphenyl)-, acetate (9CI) (CA INDEX NAME)



L50 ANSWER 185 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1960:91693 HCAPLUS

DOCUMENT NUMBER: 54:91693

ORIGINAL REFERENCE NO.: 54:17384f-i,17385a-d

TITLE: Anthoxanthins. IX. Syntheses of the fourth racemate of a flavan-3,4-diol and isomeric catechins

AUTHOR(S): Kashikar, M. D.; Kulkarni, A. B.

CORPORATE SOURCE: Inst. Sci., Bombay

SOURCE: Journal of Scientific & Industrial Research (1959), 18B, 413-17

CODEN: JSIRAC; ISSN: 0022-4456

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. CA 52, 5397e; 53, 11358b. The 4th racemate of 6-methyl-4'-methoxyflavan-3,4-diol (I) was synthesized by hydrogenating the corresponding flavanol over Raney Ni. Hydrogenation being erratic (King and Clark-Lewis, CA 50, 7785g) a catechin was often formed; this was isolated and characterized. Derivs. of the flavanol were reduced under milder conditions (avoiding hydrogenolysis) to give I. Two isomeric 6-methyl-3,4'-dimethoxyflavan-4-ols were obtained, corresponding to both possible isomers of the catechin. The CrO₃-C₅H₅N complex showed promise as a reagent for the stereochemical investigation of cyclic glycols. Hydrogenation of 2 g. 6-methyl-4'-methoxyflavanol (II) with 4 g. Raney Ni in 50 ml. EtOH 16 hrs. at 100-10° and 100 atmospheric gave 0.2 g. I, m. 162°. Mixed m.p. with the 1st racemate (m. 169°) was depressed to 142.5°. Acetylation of I gave the diacetate, m. 128-9°. Mixed m.p. of this diacetate with diacetate of 1st racemate was depressed to 106-8°. Hydrogenation of 2 g. II with 3-4 g. Raney Ni in 400 ml. EtOH 20 hrs. at 110-20° at 600 lb./sq. in. gave 6-methyl-4'-methoxyflavan-3-ol m. 135°; acetate m. 150°. A mixture of 0.4 g. 6-methyl-4'-methoxyflavanol Me ether (III), 60 ml. EtOH, and 0.2 g. NaBH was refluxed 5 hrs., cooled, and hydrogenated with 0.2 g. Raney Ni 7 hrs. at room temperature at 45 lb./sq. in. to give 0.06 g. 6-methyl-3,4'-dimethoxyflavan-4-ol (IV), m. 187-8°. It gave a violet color with concentrated H₂SO₄, while the starting material

gave a greenish yellow fluorescence. A solution of 0.4 g. LiAlH₄ in 120 ml. Et₂O was added to 0.4 g. III in 30 ml. C₆H₆ and 20 ml. Et₂O, the mixture cooled,

allowed to stand 2 hrs., and hydrogenated with 0.2 g. Raney Ni 7 hrs. at room temperature at 45 lb./sq. in. to give IV; acetate m. 107-9°. A mixture of 0.6 g. 6-methyl-3,4'-dimethoxyflavanol 4-acetate in 40 ml. EtOH and 10 ml. 10% Na₂CO₃ was refluxed 1 hr., cooled, diluted with H₂O, and extracted repeatedly with Et₂O. The extract gave 0.3 g. isomeric 6-methyl-3,4'-dimethoxyflavan-4-ol, m. 106-8°. Benzoylation of 0.564 g. II with 0.3 ml. BzCl and 0.2 ml. C₅H₅N at 0-5° gave 0.5 g. II benzoate, m. 168-70°. Treatment of 0.5 g. LiAlH₄ in 150 ml. dry Et₂O with 0.5 g. II benzoate in 50 ml. dry C₆H₆ 2 hrs., followed by hydrogenation with 0.3 g. Raney Ni 7 hrs. at room temperature and 45 lb./sq.

in.

gave 0.15 g. 6-methyl-4'-methoxyflavan-3-ol (V), m. 120-1°, violet color with concentrated H₂SO₄. Acetylation of 0.05 g. V with Ac₂O and C₅H₅N gave 0.03 g. V acetate, m. 141-2°. Hydrogenation of 0.5 g.

6-methyl-4'-methoxydihydroflavanol acetate in 50 ml. EtOH with 0.3 g. Raney Ni 4 hrs. at room temperature at 45 lb./sq. in. gave 0.41 g.

6-methyl-4'-methoxy-3-acetoxyflavan-4-ol (VI), m. 182-3°, violet color with concentrated H₂SO₄. Hydrolysis of 0.075 g. VI in 15 ml. EtOH by refluxing 1 hr. with 10 ml. 10% Na₂CO₃ gave 0.04 g. 1st racemate of I, m.

160° (mixed m.p.). Benzoylation of 1 g. VI with 0.8 ml. BzCl and 2 ml. C₅H₅N at 0.5° gave 0.9 g. 6-methyl-4'-methoxy-3-acetoxy-4-benzoyloxyflavan, m. 156-7°, violet color with concentrated H₂SO₄. A solution of the 1st racemate of I (0.3 g., m. 169°) in 3 ml. C₅H₅N was added to a slurry of 0.3 g. Cr₂O₃ and 3 ml. C₅H₅N, shaken vigorously, allowed to stand overnight at room temperature, diluted with H₂O, extracted

repeatedly

with Et₂O, and the extract washed with dilute HCl and H₂O. The extract gave

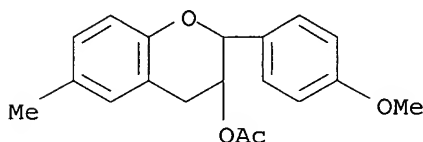
0.15

g. 6-methyl-4'-methoxydihydroflavanol, m. 160°. When the 2nd racemate of I, m. 193°, was treated in a similar manner the same dihydroflavanol was obtained.

IT 851-80-9, 3-Flavanol, 4'-methoxy-6-methyl-, acetate
(preparation of)

RN 851-80-9 HCAPLUS

CN 3-Flavanol, 4'-methoxy-6-methyl-, acetate, cis- (8CI) (CA INDEX NAME)



L50 ANSWER 186 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1960:62708 HCAPLUS

DOCUMENT NUMBER: 54:62708

ORIGINAL REFERENCE NO.: 54:12128d-i

TITLE: Stereochemical relations in the flavonoid group

AUTHOR(S): Weinges, Klaus

CORPORATE SOURCE: Univ. Heidelberg, Germany

SOURCE: Ann. (1959), 627, 229-36

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The configuration of some naturally occurring, optically active dihydroflavonols and 3,4-flavandiols was that of (+)- or (-)-catechin with H atoms on C-2 and C-3 in trans position. The existence of epidihydroflavonols in nature was questioned. Fresh shavings of Rhus

glabra wood were extracted with ether for several days, the extract was concentrated to

200 ml., and followed by countercurrent distribution with H₂O as the 2nd phase to yield after 200 transfers in tubes 140-70 crystalline dl-fustin, m. 223-5°, [α]_D25 \pm 0° (acetone-H₂O).

Tetraacetyl-dl-fustin, m. 147-8° (MeOH), with H₂-Pt in EtOAc yielded 3,3',4',7-tetraacetoxy-4-hydroxyflavan, m. 188-90° (MeOH).

Acetylation gave 3,3',4,4',7-pentaacetoxyflavan, m. 122-4° (MeOH).

dl-3',4',7-Trihydroxy-3,4-flavandiols with H₂-Pd in dioxane gave

dl-3',4',7-trihydroxy-3-flavanol, m. 212-14° (H₂O), which with

Me₂SO₄ and 50% KOH gave dl-3',4',7-trimethoxy-3-flavanol, m.

121-3°. (-)-Fustin, m. 216-18°, [α]_D25 -26°

(1:1 acetone-H₂O), and (-)-3',4',7-trihydroxy-3,4-flavandiols were isolated

from *Cotinus coggygria* wood; tetraacetyl-(-)-fustin m. 117-18°.

Hydrogenation of (-)-fustin yielded (+)-3',4',7-trihydroxy-3-flavanol, m.

208-11°, [α]_D25 10.1° (1:1 acetone-H₂O);

(-)-3,3',4',7-tetraacetoxyflavan m. 96-8° (EtOH), [α]_D25

-2.4° (C₂H₂Cl₄). Optically impure 3',4',5,7-tetramethyltaxifolin,

obtained from (+)-taxifolin with Me₂SO₄ and K₂CO₃ in dry acetone, m.

170-2°; acetylation with Ac₂O and pyridine gave

3',4',5,7-tetramethyl-3-acetyl-dl-taxifolin, m. 184°, reduction of

which with LiAlH₄ in tetrahydrofuran gave dl-3',4',5,7-tetramethoxy-3,4-

flavandiols, m. 204-6°; this with Ac₂O in pyridine gave the

3,4-diacetate, m. 133-5° (MeOH). (-)-3',4',5',7-Tetramethoxyflavan-

3-phenylglyoxylate, obtained from 2.2 g. 3',4',5',7-tetramethoxy-3-

flavanol and 2.8 g. phenylglyoxyl chloride in 8 ml. pyridine and 12 ml.

benzene, m. 94-6°, [α]_D25 -6.4° (C₂H₂Cl₄). By the

procedure of Birch, et al. (C.A. 52, 4614b), 600 mg. phenylglyoxylate

yielded 340 mg. (-)-3',4',5',7-tetramethoxy-3-flavanol and 120 mg.

atrolactic acid, m. 76-84°, [α]_D25 -2.3° (EtOH).

IT 115760-12-8, Glyoxylic acid, phenyl-, L-2-(3,4-dimethoxyphenyl)-

5,7-di-methoxy-3-chromanylester 857402-06-3, 3-Flavanol,

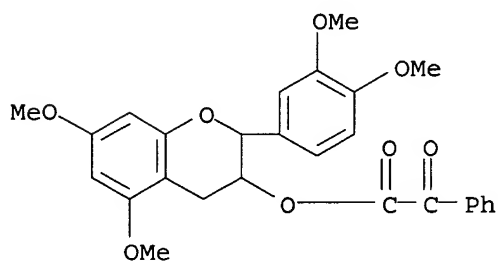
3',4',5',7-tetramethoxy-, phenylglyoxylate

(preparation of)

RN 115760-12-8 HCAPLUS

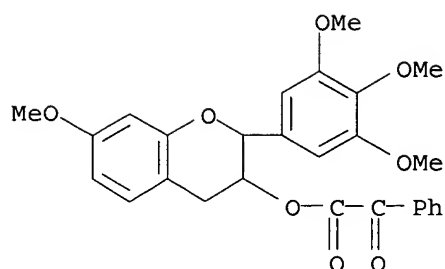
CN Glyoxylic acid, phenyl-, L-2-(3,4-dimethoxyphenyl)-5,7-dimethoxy-3-

chromanylester (6CI) (CA INDEX NAME)



RN 857402-06-3 HCAPLUS

CN 3-Flavanol, 3',4',5',7-tetramethoxy-, phenylglyoxylate (6CI) (CA INDEX NAME)



L50 ANSWER 187 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1959:105525 HCAPLUS

DOCUMENT NUMBER: 53:105525

ORIGINAL REFERENCE NO.: 53:18948e-h

TITLE: Black wattle catechin

AUTHOR(S): Roux, D. G.; Maihs, A. E.

CORPORATE SOURCE: Rhodes Univ., Grahamstown, S. Afr.

SOURCE: Nature (London, United Kingdom) (1958), 182, 1798

CODEN: NATUAS; ISSN: 0028-0836

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 52, 19202a. Ultraviolet examination and anhydrous alkaline degradation of

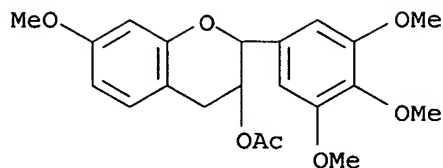
condensed tannins from *Acacia mollissima* bark suggested the catechin structure, 3,7,3',4',5'-pentahydroxyflavan as a possible prototype of many of the complex tannins present in black wattle extract, and the pure crystalline

constituents G (I), H (II), A2 (III) of wattle tannins have been shown to rank as major catechin components of the extract. Color reactions and degradation products of II, m. 205-7°, $[\alpha]_{20D} -10.7^\circ$, λ 203,281 m μ in the assumed flavan indicated the presence of only pyrogallol and resorcinol nuclei and chromatographic behavior suggested the probable presence of 5 HO groups (4 phenolic, 1 aliphatic) as demonstrated by formation of an O-tetra-Me derivative, m. 140-1°, $[\alpha]_{20D} -21.6^\circ$, and its mono-Ac derivative, m. 73°. II and (-)-robinetinidol (IV) (Weinges, C.A. 53, 4264g) showed no mixed m.p. depression, had identical infrared absorption in the 2.5-15 μ range and gave identical R_f values in 3 solvent systems. Chromatographic evidence also suggested the presence of an epimeric 2,3-cis-substituted IV in wattle extract. This 1st recorded isolation of a catechin of the resorcinol series also suggested the natural occurrence of (+)-robinetinidol in apparent contrast to the catechins of the phloroglucinol series where mainly (-)-epi- and (+)-forms occur in plants. The tentative identification of I and III as (+)-catechin and (+)-gatlocatechin, (C.A. 47, 11785f) was confirmed by isolation and comparison with the same compds. from *Casuarina equisetifolia* (C.A. 51, 18480h).

IT 100736-00-3, 3-Flavanol, 3',4',5',7-tetramethoxy-, acetate (preparation of)

RN 100736-00-3 HCAPLUS

CN 3-Flavanol, 3',4',5',7-tetramethoxy-, acetate (6CI, 7CI) (CA INDEX NAME)



L50 ANSWER 188 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1959:23290 HCAPLUS
 DOCUMENT NUMBER: 53:23290
 ORIGINAL REFERENCE NO.: 53:4264g-i,4265a-e
 TITLE: Catechins and their formation from leucoanthocyanidin hydrates
 AUTHOR(S): Weinges, Klaus
 CORPORATE SOURCE: Univ. Heidelberg, Germany
 SOURCE: Ann. (1958), 615, 203-9
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB cf. C.A. 52, 18383f. The nomenclature used is that described previously (loc. cit.). By hydrogenating various leucoanthocyanidin hydrates with Pd in dioxane the OH group on the 4-C atom was eliminated with the formation of 50-70% corresponding catechin. This represents a new and satisfactory catechin synthesis. A method is also given for isolating from Douglas fir the hitherto difficultly obtainable (-)-epicatechin (I). PdCl₂ (0.7 g.) in 30 cc. MeOH hydrogenated, the resulting Pd added to 2 g. leucofisetidin hydrate in 50 cc. warm dioxane, hydrogenated 16 hrs. with gradual cooling to 20°, and the filtered mixture evaporated in vacuo gave 1.3 g. (+)-fisetidinol (3',4',7-trihydroxy-3-flavanol) (II), m. 208-11° (H₂O), [α]_D²⁵ 10.1° (c 2, 1:1 Me₂CO-H₂O). Unless otherwise stated, all other [α]_D²⁵ were taken in (CHCl₂)₂ (c 2). II in MeOH with Me₂SO₄ and 50% KOH gave the 3',4',7-tri-Me ether (III), m. 119-20° (MeOH), [α]_D^{30.5} III (0.9 g.) in 6 cc. HCONMe₂ containing 0.75 g. MeI shaken 12 hrs. with 0.75 g. Ag₂O, centrifuged, washed thoroughly with CHCl₃, and the combined organic solns. washed with H₂O, dried, and evaporated gave the 3-Me ether of III, m. 80-2°, [α]_D^{19.2}. III (0.5 g.) with Ac₂O and pyridine kept 3 hrs. at 50° and poured on ice gave the 3-acetate of III, m. 90-1°, [α]_D^{20.4}. Similarly III with mesyl chloride and pyridine at -20° then 16 hrs. at 0° gave the 3-mesyl ester of III, m. 108-10° (MeOH with C), [α]_D^{-14.2}. Similarly at 100° was formed the 3-tosyl ester of III, m. 129-30°, [α]_D^{-69.1}. When, by a slight modification of the Freudenberg-Hartmann method (C.A. 49, 5456g), Robipia pseudacacia wood meal was percolated with Me₂CO, concentrated to small volume, crystals separated

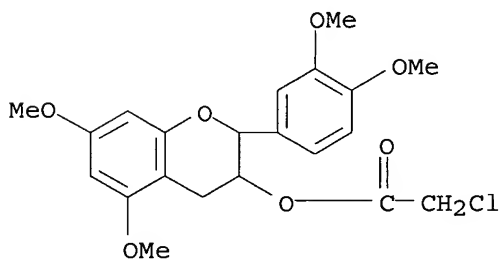
at 0°. The filtered product in 200 cc. H₂O was freed from Me₂CO and fractionated by countercurrent partition with Et₂O as the 2nd phase. After 135 stages, (+)-dihydorobinetin, [α]_D²⁵ 29° (c 2, 1:1 Me₂CO-H₂O), was obtained from the aqueous phase of tubes 30-75 by evaporation in vacuo; this was converted into leucorobinetinidin hydrate, which hydrogenated as above gave (-)-robinetinidol (3',4',5',7-tetrahydroxy-3-flavanol) (VI), C₁₅H₁₄O₆·2H₂O, m. 207-9°, [α]_D²⁵ -11.5° (c 2, 1:1 Me₂COH₂O), losing 1 mol. H₂O at 50°/12 mm. over P₂O₅ and giving anhydrous IV at 100°/1 mm. with gradual pink discoloration. The 3',4',5',7-tetra-Me ether (V) of IV m. 140-1° (EtOH), [α]_D^{-22.3}; 3-Me ether of V m. 104-5° (EtOH),

[α]D -12.2°; 3-acetate of V m. 73-5° (dilute EtOH),
 [α]D -15.2°; 3-mesyl ester of V m. 130-1° (MeOH),
 [α]D 8.7°; and 3-tosyl ester of V m. 124-5°,
 [α]D 83.7°. Fresh air-dried powdered bark of *Pseudotsuga*
taxifolia (3 kg.) was extracted 24 hrs. with C₆H₆, the evaporated extract
 reextd. 3
 days with Et₂O, this extract evaporated to 250 cc., and added to the 1st 10
 tubes
 of a countercurrent partition apparatus, the 2nd phase being H₂O. After the
 initial 100 stages, 4-5 g. taxifolin, m. 237-9°, [α]25D
 42° (c 2, Me₂CO-H₂O), had been separated completely from the catechins.
 Monitored by paper chromatograms, 500 more stages were required before 5-6
 g. (+)-catechin (VI) (somewhat contaminated by DL-catechin) was separated from
 1-2 g. I. The 3',4',5,7-tetra-Me ether (VII) of VI m. 143-4°
 [α]D -13.6°. The following 3-(O-derivs.) of VII are
 described: Ac, m. 95-6°, [α]D 6-8°; Me, m.
 93-4° [α]D 8.2°; mesyl, m. 137-8°, [α]D
 21.6°; tosyl, m. 110-11°, [α]D 92.4°; PhCH₂, m.
 105-7°, [α]D 36.5°; EtCO, m. 95-7°, [α]D
 12.0°; Bz, m. 114-16°, [α]D 25.7°; ClCH₂CO, m.
 129-31°, [α]D 17.3°. The 3',4',5,7-tetra-Me ether
 (VIII) of I m. 154-6°, [α]D -61.0°. The following
 3-(O-derivs.) of VIII were prepared: Ac, m. 104-6°, [α]D
 -72.5°; Me, m. 103-4°, [α]D -84.0°; mesyl, m.
 147-8°, [α]D -50.2°; and tosyl, m. 167-9°,
 [α]D -16.9°. Other derivs. of VIII (analogs of those prepared
 from VII) could not be crystallized 25 references.

IT 102448-90-8, Acetic acid, chloro-, 2-(3,4-dimethoxyphenyl)-5,7-
 dimethoxy-3-chroman-yl ester 102475-63-8, Propionic acid,
 2-(3,4-dimethoxyphenyl)-5,7-dimethoxy-3-chroman-yl ester
 (preparation of)

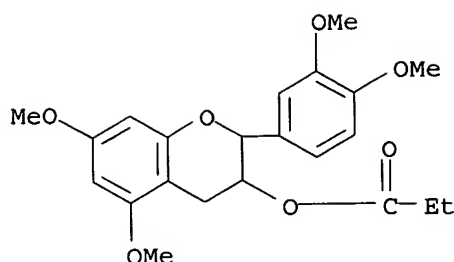
RN 102448-90-8 HCAPLUS

CN Acetic acid, chloro-, 2-(3,4-dimethoxyphenyl)-5,7-dimethoxy-3-chroman-yl
 ester (6CI) (CA INDEX NAME)



RN 102475-63-8 HCAPLUS

CN Propionic acid, 2-(3,4-dimethoxyphenyl)-5,7-dimethoxy-3-chroman-yl
 ester (6CI) (CA INDEX NAME)



L50 ANSWER 189 OF 189 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1948:2601 HCAPLUS

DOCUMENT NUMBER: 42:2601

ORIGINAL REFERENCE NO.: 42:559c-f

TITLE: A glucoside from *Gleditsia triacanthos*

AUTHOR(S): Gakhokidze, A. M.

CORPORATE SOURCE: Chem. Inst., Georgia (U.S.S.R.) Acad. of Sci.

SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian

Federation) (1946), 19, 1197-1200

CODEN: ZPKHAB; ISSN: 0044-4618

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Pulverized seeds (5 ks.) of *Gleditsia triacanthos* (honey locust) (I) were extracted with 18 l. boiling 90% EtOH, the extract was treated with Pb(OAc)₂ and

3% aqueous HCl, filtered, concentrated to 400 ml. under reduced pressure, and diluted

with 400 ml. H₂O; the resultant precipitate was extracted with EtOAc, the EtOAc was

evaporated, and the residue was taken up in EtOH and precipitated with H₂O to give

9.5 g. 1-epicatechol 3-D-glucoside dihydrate (II), m. 259°, converted to the anhydrous form (III) by drying in vacuo. II was converted to the octaacetate of III, m. 216° (from EtOH). II (3.6 g.) in 150 ml. Me₂SO₄ at 60°, treated with a slight excess of 25% aqueous NaOH and the mixture heated 2 hrs. at 100° and extracted with CHCl₃, yielded a partially methylated derivative which, on further treatment with MeI and Ag₂CO₃, gave the octa-Me derivative (IV) of III, m. 192-3° (from MeOH), [α]_D²⁰ 42.7° (in MeOH). II (2.1 g.), refluxed 4 hrs. with 500 ml. of 2% aqueous H₂SO₄, the hot solution neutralized with BaCO₃, filtered, concentrated to 100 ml., and cooled, gave crystalline 1-epicatechol

(characterized by

its pentaacetate and penta-Me ether) and an aqueous solution of D-glucose, isolated as the phenylosazone. Refluxing 2.8 g. IV in 100 ml. 5% H₂SO₄ 6 hrs. gave on cooling crystalline 3',4',5,7-tetramethyl-1-epicatechol, which formed the known 3-Ac derivative. The filtrate contained 2,3,4,6-tetramethyl-D-glucose, identified as the anil. It was possible to extract 1.3% free glucose from I with boiling water.

IT 58065-34-2, Epicatechol, 3',4',5,7-tetramethyl-, 3-acetate (preparation of)

RN 58065-34-2 HCAPLUS

CN 2H-1-Benzopyran-3-ol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-5,7-dimethoxy-, acetate, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

